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Bongaerts, J.H.H.

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Chapter 4

Propagation of a partially coherent focused x-ray beam within a planar x-ray waveguide

This chapter is based on the article entitled 'Propagation of a partially coherent focused x-ray beam within a planar x-ray waveguide', which appeared in the Journal of Synchrotron Radiation [37].

4.1 Introduction

The sample size of an ultrathin fluid confined within the planar x-ray waveguide is very small and so are its refractive-index contrasts. Therefore, an x-ray beam of high flux density is necessary in order to be sensitive to the refractive-index contrasts of the fluid in a scattering experiment. Even at a third-generation synchrotron facility, like the ESRF, the scattered intensity can be too low. Since the vertical width of an unfocused x-ray beam at a synchrotron facility is much larger (\(\sim 0.5\) mm in our case) than the waveguide width \(W\) (typically \(W < 1\) \(\mu\)m), most of the available flux is wasted if the waveguide modes are excited from the side, as described in section 2.2.2. If the unexploited flux were to be made available to the waveguide, a wider range of diffraction studies on samples with a low refractive-index contrast would be possible. Furthermore, the transverse coherence length along the vertical direction, \(\xi_v \sim 100\) \(\mu\)m, is much larger than the waveguide gap width \(W\). By matching \(\xi_v\) to \(W\), a large flux enhancement can be achieved without significantly affecting the degree of coherence of the e.m. waves inside the waveguide.

Here, we attain the flux enhancement by pre-focusing the incident beam onto
Figure 4.1: Schematic of the waveguide setup with the pre-focusing lens (not to scale). The guiding layer of the waveguide is the gap in between the two closely spaced surfaces on the right. The dark layers in the substrates are the aluminum layers that form the optical interferometer for the FECO technique (see text). The incident beam is focused on the entrance of the waveguide by a transmission Fresnel zone plate lens, which can be removed. By rotating the lens around the axis indicated by the dashed line the effective path length through the Fresnel zones can be adjusted to achieve optimal efficiency.
the entrance of the waveguide with a one-dimensional diffractive lens (see Fig. 4.1). This creates a narrow line focus at the entrance of the waveguide. This approach is different from that in earlier experiments, where a resonant beam coupler (RBC) was employed to excite the waveguide modes [38, 39, 40]. In the RBC scheme the flux enhancement is achieved by exciting the waveguide modes via an evanescent wave through a thin upper boundary layer. In this way a larger part of the incident beam is used. In our setup, however, the waveguide boundaries are thick slabs of silica, which will scatter and absorb the incident beam, rendering the RBC-scheme ineffective. Furthermore, a disadvantage of the RBC is the fact that the modes that have been excited in the waveguide are constantly leaking out through the thin upper boundary layer.

In this chapter we present experiments in which a significant flux enhancement in the waveguide is achieved by pre-focusing of the x-ray beam. We examine the effects of the beam compression on the propagation of the waveguide modes through the waveguide. In section 4.2 the lens is discussed. The propagation of a partially coherent beam through the waveguide is described in section 4.3 by way of the mutual intensity function. section 4.4 discusses the experimental procedures and the results are shown in section 4.5. A conclusion and brief outlook are given in section 4.6.

4.2 Fresnel zone plate lens

The incident beam is focused onto the entrance of the waveguide by a one-dimensional transmission Fresnel zone plate (FZP) with its zones parallel to the waveguide plane. An example of such a FZP lens is shown in the scanning electron micrograph of Fig. 4.2. It consists of a rectangular pattern of trenches and ridges with a 50% duty cycle (trench-to-ridge ratio of 1:1) on a 5 μm thick silicon membrane. The membrane was home-made by reactive ion etching [41]. The width of the Fresnel zones (71 zone pairs in total) decreases away from the center and the outermost zone width \( d \) is 350 nm. The height \( h \) of the ridges is 5.5 μm. The lens aperture perpendicular to the ridges, \( D \), equals 200 μm and along the ridges 2.5 mm. The structure was patterned by use of electron-beam lithography and subsequently wet chemical etching. Details of the manufacture process are given in Ref. [41].

The focusing efficiency of the FZP lens depends on the shape and height of the zone plate structures. For a structure with a rectangular profile and a 50% duty cycle, the first-order diffraction peak has a maximum theoretical collecting
efficiency $\eta_{\text{lens}}$ given by [42]

$$
\eta_{\text{lens}} = \frac{1}{\pi^2} \left( 1 + e^{-2\phi\beta/\delta} - 2e^{-\phi\beta/\delta} \cos(\phi) \right),
$$

(4.1)

where $\delta$ and $\beta$ represent the real and imaginary part of the refractive index $n = 1 - \delta + i\beta$, respectively, and $\phi = 2\pi h\delta/\lambda$ is the relative phase shift between the x rays travelling through the ridges and those travelling through the trenches. The efficiency is at a maximum for $\phi \approx \pi$. In our case, the wavelength $\lambda$ equals 0.0939 nm and the lens material is silicon, yielding $\delta_{\text{Si}} = 2.79 \cdot 10^{-6}$ and $\beta_{\text{Si}} = 2.44 \cdot 10^{-8}$. This gives an optimum zone height, $h$, of 16.8 $\mu$m, which is significantly larger than the fabricated structure height of 5.5 $\mu$m. However, by rotating the lens by an angle of 70.9° with respect to the x-ray beam (see Fig. 4.1) we increase the effective path length $h$ through the ridges to 16.8 $\mu$m. In this way, the lens can be used at energies typically between 8 and 15 keV, each energy having its own optimal efficiency angle [43]. The efficiency of the $+1^{st}$ order diffraction maximum of a perfect zone-plate lens is in our case 39.5%. The absorption length in silicon at $\lambda = 0.0939$ nm is 303 $\mu$m and when taking into account the absorption in
4.3 Coherent properties of the beam

We now describe the coherent properties of the beam as it propagates via the lens and the waveguide to the detector. For this purpose we introduce the mutual intensity function \( J(x, x') \) [13], which contains both the intensity distribution of the electric field, via \( I(x) = J(x, x) \), and the complex degree of coherence between the electric fields at two different points \( x \) and \( x' \) in a plane \( S \), perpendicular to the propagation direction. The complex degree of coherence \( \mu(x, x') \) is defined as

\[
\mu(x, x') = \frac{J(x, x')}{\sqrt{I(x)I(x')}}. \tag{4.2}
\]

If the mutual intensity function \( J_i(x_i, x_i') \) at one plane \( S_i \) is known, its propagation to a next plane \( S_j \) is calculated via

\[
J_j(x_j, x_j') = \iint dx_i dx_i' J_i(x_i, x_i') K_{ij}(x_i, x_j) K_{ij}^*(x_i', x_j'), \tag{4.3}
\]

where \( K_{ij}(x_i, x_j) \) is the transmission function describing the electric field at \( x_j \) in the plane \( S_j \) as a function of the field at \( x_i \) in the plane \( S_i \), and \( K_{ij}^* \) is the complex conjugate of \( K_{ij} \). We propagate the mutual intensity function (MIF) from the source to the FZP lens, then to the waveguide and finally to the detector plane (see Fig. 4.3). In this way we obtain the intensity distribution at the detector for a partially coherent focused beam. A step-by-step description of the propagation of the MIF from the source to the detector can be found in Appendix A, a summary of which is given below.

We assume a completely incoherent source with a Gaussian intensity profile \( I_s(x_0) \) in the vertical \( x \)-direction, given by

\[
I_s(x_0) = A_0 \exp \left(- \frac{x_0^2}{2\sigma_{0,v}^2} \right). \tag{4.4}
\]

In the horizontal direction, the source is much larger than in the vertical direction and is considered to be infinite in the calculations. This allows a two-dimensional
Figure 4.3: Schematic of the setup with the x-ray source, lens, waveguide and detector. The lens aperture can be set by an adjustable horizontal slit in front of the lens. Five planes $S_i$ are defined, as well as the distances $R_{ij}$ between the source, lens, waveguide and detector. The distance between a point $x_i$ in plane $S_i$ and $x_j$ in plane $S_j$ is depicted by $s_{ij}$. The subscripts $i$ in the coordinates $x_i$ in the text refer to the subscripts of the corresponding planes $S_i$. Angles and distances are not to scale.

Propagation of the e.m. field in cylindrical waves and the vector $x_i$ is replaced by the scalar $x_i$. After propagation through empty space, the absolute value of the degree of coherence $|\mu_i(x_i, x'_i)|$ at a distance $R_{0i}$ away from the source is then given by

$$|\mu_i(x_i, x'_i)| = \exp\left(-\frac{2\pi^2\sigma_{0,z}^2(x_i - x'_i)^2}{\lambda^2 R_{0i}^2}\right).$$

The vertical coherence length $\xi_{i,v}$ at a distance $R_{0i}$ is given by

$$\xi_{i,v} = \frac{\lambda R_{0i}}{s_{0,v}},$$

where $s_{0,v} = 2\sqrt{2\ln(2)}\sigma_{0,v}$ is the full-width-at-half-maximum (FWHM) of the intensity profile of the source. The transverse coherence lengths in the planes $S_i$ are denoted in the remainder of the text by $\xi_{i,v}$ and $\xi_{i,h}$ for the vertical and horizontal direction, respectively.

By treating the FZP lens as an ideal phase-shifting lens, we greatly simplify our calculations. The coherence length in the image plane $S_3$ can be found by solving the integral given for the mutual intensity function $J_3(\theta_i, x_3, x'_3)$ at the waveguide entrance, where $\theta_i$ is again the incidence angle. We do not show the result here, since it is rather elaborate. Instead, we estimate the coherence length as follows. The source may be divided in $N$ parts that all illuminate the lens coherently (Fig. 4.4). The size $s_{0,v}^{coh}$ of such a part is given by the equation $D = \xi_{1,v}$, which gives $s_{0,v}^{coh} = \lambda R_{01}/D$. Every such part of the source is effectively a point source for this imaging system and sets the resolution of the imaging system in the object.
4.3. Coherent properties of the beam

The source can be divided into small parts of size \( S_{0,v}^{\text{coh}} \) such that every sub-source illuminates the lens coherently. A source of this size can be considered to be a point source and will have a fully coherent image. The size of this image is determined by the resolution of the lens \( d_f \).

Figure 4.4: The source can be divided into small parts of size \( S_{0,v}^{\text{coh}} \) such that every sub-source illuminates the lens coherently. A source of this size can be considered to be a point source and will have a fully coherent image. The size of this image is determined by the resolution of the lens \( d_f \).

plane \( S_0 \). This point source results in a coherent image of size \( d_f \), being the resolution of the lens in the image plane \( S_3 \). Therefore, the coherence length in the image plane \( \xi_{3,v} \sim d_f \) in the presence of the lens, which is much smaller than the coherence length at the waveguide in the absence of the lens. Without showing the details here, we mention that the argument above is in agreement with numerical evaluations of the MIF at the image plane \( J_5(\theta_i, x_3, x'_3) \) (see Appendix B). These showed that the coherence length in the image is, within a factor of two, equal to the resolution of the imaging system \( d_f \), namely \( \xi_{3,v}^{\text{FZP}} \sim 1.8d_f \).

After propagating the mutual intensity function from the source to successively the lens, the waveguide and the detector plane \( S_5 \), we find that \( J_5(\theta_i, x_5, x'_5) \) is given by (Appendix A)

\[
J_5(\theta_i, x_5, x'_5) = A_5 \iint_{\text{lens}} dx_2 dx'_2 \exp \left( \frac{-2\pi^2 \sigma_{0,v}^2 (x_2 - x'_2)^2}{\lambda^2 R_{01}^2} \right) \times E_x^p(\theta_i + \frac{x_2}{R_{23}}, x_5) E_x^o(\theta_i + \frac{x'_2}{R_{23}}, x'_5),
\]

where the integration boundaries are given by the lens aperture, the pre-factor \( A_5 = A_0 4\sqrt{2\pi} \sigma_{0,v}/(\lambda R_{01} R_{23}) \), and \( R_{01} \) and \( R_{23} \) are the distances between the source and the lens and between the lens and the waveguide, respectively. The e.m. field \( E_x^p(\theta_i + x_2/R_{23}, x_5) \) is the field in the detector at the point \( x_5 \) due to a plane wave of unit amplitude, incident onto the waveguide at an angle \( \theta_i + x_2/R_{23} \).

Therefore, the propagation of the partially coherent focused beam through the
waveguide can be described by a combination of incident plane waves. Once the e.m. field $E^p_5(\theta_i, x_5)$ is numerically evaluated in the relevant range of incidence and exit angles (the exit angle $\theta_e \simeq x_5/R_45$), the mutual intensity function can be calculated for various source sizes $\sigma_{0,e}$. Since the numerical evaluations of the propagation of the e.m. field through the waveguide are very time consuming, this speeds up the analysis significantly. Lens defects are described statistically by multiplying the propagator $E^p_5(\theta_i + x_2/R_{23}, x_3)$ by a focusing-efficiency function $F(x_2)$.

We now discuss briefly the two extreme cases of complete incoherent and complete coherent illumination of the lens. In the limit of an infinitely large source, the lens is illuminated by fully incoherent radiation. The Gaussian function in Eq. 4.7, which is identical to the absolute value of the degree of coherence at the lens exit $|\mu_2(x_2, x_2')|$, can then be replaced by $\lambda R_{01}/(\sqrt{2\pi} \sigma_{0,e})$ times the Dirac delta function $\delta(x_2 - x'_2)$. This gives us the intensity distribution $I_5^{\text{incoh}}(\theta_i, x_5)$ in the detector plane for incoherent illumination of the lens:

$$I_5^{\text{incoh}}(\theta_i, x_5) = A_0 \frac{4}{R_{23}} \int_{\text{lens}} dx_2 \left| E^p_5(\theta_i + \frac{x_2}{R_{23}}, x_5) \right|^2.$$

(4.8)

In the case of coherent illumination of the lens, the source size $\sigma_{0,e}$ can be set to zero and the intensity distribution $I_5^{\text{coh}}(\theta_i, x_5')$ is given by

$$I_5^{\text{coh}}(\theta_i, x_5) = A_0 \iint_{\text{lens}} dx_2 dx'_2 E^p_5(\theta_i + \frac{x_2}{R_{23}}, x_5) E^p_5(\theta_i + \frac{x'_2}{R_{23}}, x_5).$$

(4.9)

For coherent illumination of the lens, the interference effects between the different modes will be largest and this will result in large intensity modulations in the diffraction patterns in the detector. In the case of incoherent illumination, the intensity modulations will be small.

### 4.4 Experimental

The waveguide studied in this chapter consists of a lower silica disk with a diameter of 25.4 mm and an upper silica disk with a diameter of 5.5 mm. The surfaces of the disks are coated with a 30 nm thick aluminum layer and a 650 nm thick silica spacer layer on top. The r.m.s. roughness of the top silica surface is below 1 nm. The air gap between the opposing silica surfaces forms the x-ray guiding layer (see chapter 3).

The experiment was performed at the ID22 undulator beam line of the European Synchrotron Radiation Facility (ESRF) in Grenoble. The lens, the waveguide setup and the detectors were all positioned on a single granite optical table. This
provided the necessary stability of the relative positions of the components. The distances between the lens and the source and the lens and the waveguide were $R_{01} = 40 \text{ mm}$ and $R_{23} = 760 \text{ mm}$, respectively. At these positions, the lens images the source height exactly onto the waveguide entrance with a magnification factor $M = R_{23}/R_{01} \approx 1/52.6$. An adjustable horizontal slit was positioned just in front of the lens in order to be able to change the lens aperture (see Fig. 4.3).

The energy of the x rays was 13.2 keV ($\lambda = 0.0939 \text{ nm}$), selected with a Si(111) double-crystal monochromator ($\Delta \lambda/\lambda = 1.4 \times 10^{-4}$). The effective vertical source size $\sigma_{v,0}$ of the undulator was experimentally determined from the visibility of the interference fringes resulting from diffraction off a thin boron fiber [44]. We found $\sigma_{v,0} = 16 \pm 1 \mu\text{m}$, which corresponds to a FWHM source size $s_{0,v} = 38 \pm 2 \mu\text{m}$. The horizontal source size equals $s_{0,h} \approx 700 \mu\text{m}$ (FWHM). The beam size at the lens was 0.5 mm along the vertical direction and 0.1 mm along the horizontal direction, defined by entrance slits. The vertical and horizontal transverse coherence lengths at the lens position equal $\xi_{1,v} \approx 99 \mu\text{m}$ and $\xi_{1,h} \approx 5.4 \mu\text{m}$, respectively. If the lens is absent, the vertical and horizontal coherence lengths at the waveguide entrance are $\xi_{3,v} \approx 101 \mu\text{m}$ and $\xi_{3,h} \approx 5.5 \mu\text{m}$, respectively.

For measurement of the total transmitted intensity through the waveguide as a function of the vertical lens position, a PIN diode was used. The PIN diode was positioned behind the waveguide and had an area large enough to capture all outgoing intensity. More detailed information is obtained from measurements of the diffracted far-field intensity distributions $I_5(\theta_i, \theta_e)$ as a function of both incidence angle $\theta_i$ and exit angle $\theta_e \approx x_5/R_{45}$. For these measurements, we used the same CCD-camera setup as described in chapter 3, now at a distance of 1180 mm from the exit of the waveguide, resulting in an angular resolution of 0.5 millidegrees. Again, by tilting the waveguide, we varied $\theta_i$ in steps of 0.001° and we obtained the diffracted intensity distribution $I_5(\theta_i, \theta_e)$ as a function of both incidence and exit angle.

### 4.5 Results

**Lens properties**

We first discuss two specific lens properties: the focusing efficiency and the size of the source image created by the lens. To measure the focusing efficiency $\eta_{\text{lens}}^1$ of the $+1^{st}$ order diffraction maximum of the zone plate lens, we set the waveguide at a gap width of $W \approx 6 \mu\text{m}$, much larger than the expected image width of $s_{3,v} = s_{0,v}M \approx 0.72 \mu\text{m}$. This is to ensure that the complete image is captured by the waveguide entrance. The waveguide was positioned in the center of the
beam and the total transmitted intensity $I(x)$ was measured as a function of the vertical lens position $x$. Thus, the focus of the first-order diffraction maximum was scanned over the entrance of the waveguide, which was tilted with respect to the beam at an angle $\theta_t = 0.02^\circ$, i.e., well below the critical angle $\theta_c = 0.125^\circ$ for the air-silica interface. The result is shown in Fig. 4.5.

The lens height is visible in Fig. 4.5 as the 200 \( \mu \)m wide low-intensity area with in its center a peak containing the flux of the +1\textsuperscript{st} order diffraction maximum. The background in the low-intensity area consists of other diffraction orders of the FZP lens. The width of the peak equals twice the waveguide width of 6 \( \mu \)m, because of the pre-reflection in front of the waveguide. The lens efficiency $\eta_{\text{lens}}$ is given by [45]

$$\eta_{\text{lens}} = \frac{1}{D I_c} \int_{\text{peak}} I(x) dx,$$  \hspace{1cm} (4.10)

where $D$ is the lens height, $I(x)$ is the total intensity transmitted through the waveguide as a function of the lens position and $I_c$ is the total transmitted intensity with the lens taken out of the beam. From the data in Fig. 4.5 and the measured
4.5. Results

Figure 4.6: The measured total transmitted intensity (diamonds connected by lines) through the waveguide as a function of the vertical lens position for a waveguide gap width $W = 244 \text{ nm}$. The FWHM of the peak, depicted by the arrow, is $1.03 \text{ \mu m}$ and the peak intensity is a factor of 54 higher than that with the lens completely removed. The dash-dotted line is a Gaussian curve of $0.84 \text{ \mu m}$ FWHM, indicating the width of the optimal theoretical curve.

value for $I_c$ we find an efficiency $\eta_{\text{lens}}$ of $32.6\%$. This is somewhat lower than the maximum theoretical focusing efficiency of $37.6\%$, given in section 4.2 for our one-dimensional zone plate lens.

Next, we closed the gap to $W \approx 244 \text{ nm}$, smaller than the expected image size $s_{3,v} = 0.72 \text{ \mu m}$, and we again scanned the vertical lens position. In this way, the waveguide is used as a narrow slit to determine the image profile. The measured transmitted intensity $I(x)$ is shown in Fig. 4.6. The FWHM of the measured peak equals $1.03 \text{ \mu m}$, which is larger than the expected image size $s_{3,v} \approx 0.72 \text{ \mu m}$ because of the limited resolution of the lens and the integration over the gap width $W$. This is taken into account by first convoluting the $0.72 \text{ \mu m}$ wide Gaussian image profile with a $(\sin(ax)/ax)^2$ function with the first zero at $x = d_f = 0.35 \text{ \mu m}$, which represents the shape of the image of a point source. This results in an image FWHM of $0.78 \text{ \mu m}$. Subsequently, we convolute the obtained image profile with a square transmission function of width $0.488 \text{ \mu m}$, which is twice the waveguide gap. The doubled width of the transmission function is a consequence of the pre-reflection in front of the waveguide. We find an expected experimental
image width of 0.84 μm (dash-dotted line in Fig. 4.6), still somewhat smaller than the measured 1.03 μm.

The maximum intensity in Fig. 4.6 is a gain factor \( G = 54 \) larger than the transmitted intensity with the lens taken out of the beam. This flux enhancement in the waveguide by almost two orders of magnitude will allow for new types of experiments on confined geometries such as photon correlation spectroscopy.

The fact that the measured efficiency is somewhat lower than the theoretical value and that the image profile is broader than theoretically expected, suggests that there are imperfections in the lens structure. Most likely, the imperfections are in the delicate outer zones, which determine the resolving power of the lens. Also, a small misalignment in the vertical tilt angle of the lens would result in a lower performance of the lens. Such a tilt changes the position-dependent phase shift \( \phi(x) \) and thereby reduces the lens efficiency. Another explanation might be that the focal spot is at a slightly different z-position for different parts of the lens, owing to its tilt angle. The z-position changes by 0.3 mm at the tilt angle used here. However, this change is much smaller than the focal depth, given by \( 2d^2/\lambda \approx 2.6 \) mm. The latter was confirmed by a measurement of the focal width at varying z-positions around the focal spot. From this we conclude that the observed broadening is not explained by de-focusing, due to the tilt angle of the lens, but mostly by small lens imperfections and a small misalignment of the lens.

Further improvements in the lens quality and alignment would enhance the gain. In the optimal case, the flux incident on the lens multiplied by the maximum efficiency of the lens \( n^l_{\text{lens}} \) would be completely focused into a Gaussian-shaped image with a FWHM of \( s_{3,r} = 0.78 \) μm (standard deviation \( \sigma_{3,r} = 0.33 \) μm). This yields a maximum theoretical gain \( G = Dn^l_{\text{lens}}/(\sqrt{2\pi}\sigma_{3,r}) = 80 \) if the gap width \( W \) is much smaller than the image size \( s_{3,r} = 0.78 \) μm.

**Propagating of a partially coherent beam through the waveguide**

Focusing of the beam results in a larger angular distribution of the beam and also affects the spatial coherence of the beam at the position of the waveguide, as mentioned in section 4.3. Furthermore, defects in the lens may have undesirable effects on the beam profile and the coherence. These effects are observable in the far-field diffraction patterns \( I_\phi(\theta_i, \theta_e) \).

We first set the waveguide at a relatively large gap width of \( W \sim 1 \) μm. The mode spacing \( \Delta\theta = \lambda/(2W) \) equals 2.7 millidegrees for this gap, which is a factor 5.5 smaller than the convergence angle of the focused beam \( \Delta\Omega = D/R_{23} = 15 \) millidegrees. This should result in the simultaneous excitation of 5 to 6 modes in the presence of the lens. Also, the coherence angle of the incident converging beam, given by \( \xi_{1,\theta}/R_{23} \approx 7.5 \) millidegrees, is of the order of a few mode spacings. By
4.5. Results

Figure 4.7: Contour plots of the far-field intensity distributions $I_5(\theta_i, \theta_e)$, as a function of the incidence and exit angles $\theta_i$ and $\theta_e$. The gap width is given by $W = 1090$ nm and the waveguide length by $R_{34} = 5.5$ mm. (a) Experimental data, without lens, (b) numerical calculation, without lens, (c) experimental data, with lens, (d) numerical calculation with lens.
studying the interference of the modes we obtain information about the coherent properties of the focused beam.

Fig. 4.7a shows a contour plot of the intensity distribution $I_5(\theta_i, \theta_e)$, measured in the absence of the lens. At angles of incidence at which the intensity has a maximum along the diagonal, the standing-wave pattern at the entrance is matched to one of the waveguide modes and only a single mode is excited. The dash-striped pattern along the diagonal is a result of multi-mode interference of neighboring modes that are excited simultaneously at angles in between mode angles [17]. The modes interfere either constructively or destructively for $\theta_e = \theta_i$, depending on both the waveguide length and the mode angles $\theta_m$. From the angular mode spacings in Fig. 4.7a, the gap width $W$ was accurately determined at $W = 1090$ nm.

We numerically simulated the measurements of the far-field diffraction patterns $I_5(\theta_i, \theta_e)$ using the beam propagation method [35] and thus obtained the e.m. field pattern $E^2_5(\theta_i, \theta_e)$ in the detector for incident plane waves (i.e., no lens inserted). The beam propagation calculations were performed on a unix-based platform by a program written in the c++ language and is based on the light numerical recipes (see Ref. [46]). Fig. 4.7b shows the numerically calculated intensity distribution $I_5(\theta_i, \theta_e)$ without lens for a waveguide gap $W = 1090$ nm and a waveguide length $R_{34} = 5.5$ mm. The agreement between the calculated and measured diffraction patterns $I_5(\theta_i, \theta_e)$ (Figs. 4.7a and 4.7b) is excellent, which demonstrates the plane-wave character and the coherence of the incident unfocused beam. The differences between Figs. 4.7a and b at angles close to zero are caused by the finite size of the lower surface both in front and at the exit of the waveguide in the experiment. The lower surface is too small to result, at small angles, in a standing-wave pattern covering the entire waveguide gap.

Fig. 4.8 shows the measured and calculated far-field diffraction patterns for one angle of incidence $\theta_i = 0.039^\circ$. Again, the agreement between calculation and experiment is good, but the minima in between the maxima are slightly deeper in the calculation than in the experiment. This is caused by small imperfections of the waveguide surfaces, which result in a filling of the minima. The surface imperfection can be either roughness, slope error or a combination of both.

Next, we inserted the lens in the beam and repeated the measurement of $I_5(\theta_i, \theta_e)$. The result is shown in Fig. 4.7c. The diagonal is now much broader than in Fig. 4.7a, which reflects the angular range of the converging cylindrical wave in the focused beam. We find an angular width of $\Delta \Omega \sim 0.015^\circ$, identical to the expected angular range.

We now apply Eq. 4.7 to calculate $I_5(\theta_i, \theta_e)$ for the case that the lens is inserted, using the numerically calculated e.m. field $E^2_5(\theta_i, \theta_e)$ for incident plane waves.
A lower focusing efficiency of the outer Fresnel zones is taken into account by multiplying the e.m. field $E^p_5(\theta_i + x_2/R_{23}, \theta_e)$ for incident plane waves by a 200 μm-wide (FWHM) square transmission profile $F(x_2)$, the rounded edges of which gradually decrease from 1 to zero within 20 μm.

We also take into account the fact that a FZP lens with a rectangular profile has many diffraction orders, of which the 1st is just the dominant one. Moreover, for every positive focusing order, there is a negative defocusing order. For all diffraction orders other than the $+1^{st}$ order the waveguide is out of focus and the beam has expanded at the waveguide position to a size much larger than the waveguide gap $W$. Therefore, only a small part enters the waveguide. This is shown in Fig. 4.9 for the positive and negative $1^{st}$-order diffraction maxima. Most of the $+1^{st}$ diffraction order will enter the 1 μm-wide waveguide, while of the negative order only a small fraction is captured by the waveguide. The angular distribution of these captured waves is much smaller than the mode spacing and they can be treated as single plane waves. Since this holds for all other diffraction
Figure 4.9: The $+1^{st}$ order diffraction maximum of the FZP lens creates a small focus at the focal point. The $-1^{st}$ order diffraction maximum results in a broad intensity distribution of size $2D$ at the focal spot. The waveguide of width $W$ only captures a fraction $W/D$ of this flux (doubled because of the pre-reflection) and the angular distribution of these waves has a width of $W/f$.

orders as well, they are indistinguishable from each other in the diffraction patterns and we will treat the contributions of all other orders collectively as a plane-wave background.

The plane-wave background is inserted in the calculations by adding to the propagator $E_5^{p}(\theta_i + x_2/R_{23}, x_5)$, used in Eq. 4.7, a plane-wave contribution only for the case $x_2 = 0$. We then have a new propagator $E_5^{p}(\theta_i + x_2/R_{23}, x_5)$, given by

$$E_5^{p}(\theta_i + \frac{x_2}{R_{23}}, x_5) = E_5^{p}(\theta_i + \frac{x_2}{R_{23}}, x_5) + B\delta(x_2)E_5^{p}(\theta_i + \frac{x_2}{R_{23}}, x_5), \quad (4.11)$$

where $\delta(x)$ is the Dirac delta function and $B\delta(x_2)$ is the amplitude of the plane wave background. Fig. 4.10 shows the measured and calculated diffraction patterns for one incidence angle $\theta_i = 0.039^\circ$. The relative intensity of the plane-wave background, given by $B^2/D^2$, was 0.1% in the calculation. The effect of the plane-wave background on the diffraction pattern is larger than this relative intensity owing to the interference term in $E_5^{p}E_5^{p*}$. The best agreement between experiment and calculation is obtained if an effective source size $s_{0,v} = 76 \, \mu m$ is assumed, twice the value given earlier in section 4.4. Since the FZP lens and the waveguide are the only added components compared to the experiment with the boron fiber from which the source size was determined earlier, they must be the origin of the enhanced effective source size. In the case without lens (Fig. 4.8), we observed small
deviations from the calculations, caused by imperfect surfaces of the waveguide.
In the experiment with the lens inserted, multiple modes are excited simultaneously and the observed intensity modulations are more sensitive to the roughness or slope error of the surfaces, resulting in an enhanced effective source size. The lens also has an effect on the effective source size but its enhancement cannot be explained by lens effects alone. If the enhanced source size was caused by the lens alone, a larger image size $s_{3,v} = 76 \, \mu m \times M = 1.46 \, \mu m$ would have been observed in Fig. 4.6.

Fig. 4.7d shows a contour plot of the calculated diffraction patterns $I_5(\theta_i, \theta_e)$ in the presence of the lens. There is a large similarity with the experimental data in Fig. 4.7c, both in the amplitude of the intensity oscillations on the diagonal, and in the narrow band of higher intensity on the diagonal. The good agreement proves that the approximation of the FZP lens by an ideal phase-shifting lens and a plane-wave background is justified.
Figure 4.11: The outgoing intensity distribution for an incidence angle $\theta_i = 0.039^\circ$, at different lens apertures. The upper curve corresponds to an aperture of 200 $\mu$m (full illumination of the lens), the middle curve to an aperture of 100 $\mu$m, and the lower curve to an aperture of 25 $\mu$m.

As discussed in section 4.3, the beam becomes partially incoherent on the length scale of the waveguide gap of 1 $\mu$m when the lens is inserted. For some experiments, however, a fully coherent beam is required. The coherence of the beam can be restored in two ways. Either the coherence length at the sample is enhanced or the sample size is reduced. The former is achieved by reducing the vertical lens aperture using an adjustable horizontal slit in front of the lens (see Fig. 4.3). In the extreme case of closing down the lens aperture to an aperture significantly smaller than the vertical coherence length $\xi_{1,v} \approx 99$ $\mu$m, the lens is illuminated by a coherent beam, which results in a coherent image at the waveguide, irrespective of its gap width $W$. Fig. 4.11 shows the far-field diffraction patterns after the waveguide for three different lens apertures ($\theta_i = 0.039^\circ$ and $W = 1090$ nm). The upper curve corresponds to full illumination of the lens with an aperture of 200 $\mu$m. The other curves correspond to a lens aperture of 100 $\mu$m (middle) and 25 $\mu$m (bottom). As the aperture is decreased, fewer modes are excited and the intensity modulations become larger. These larger modulations are a result of the enhanced
4.5. Results

Figure 4.12: The intensity distribution $J_5(\theta_i, \theta_e)$ with lens inserted and a waveguide gap of width $W_1 = 237.7$ nm at the entrance and of width $W_2 = 190.8$ nm at the exit.

degree of coherence of the beam. At an aperture of 25 \(\mu\text{m}\), the diffraction pattern is identical in shape to the curve for an incident plane wave, corresponding to fully coherent illumination of the waveguide. The differences between the lowest curve in Fig. 4.11 and Fig. 4.8 are caused by a small misalignment of the optical axis of the lens, which caused a deviation in the incidence angle $\theta_i$. Fig. 4.11 demonstrates that the coherence is maintained at a reduced lens aperture and a large gap width $W = 1090$ nm, while the intensity is a factor of two higher than the intensity for the unfocused beam. The lower gain factor here, compared to the value of 54 given earlier, is not surprising and is caused by the convolution of the image of the source with a larger square transmission profile of width 2.18 \(\mu\text{m}\), the smaller lens aperture and the fact that the FZP-lens efficiency is lower at an aperture of 25 \(\mu\text{m}\) because of the lower number of exposed Fresnel zones. At smaller gaps these effects are more favorable and the gain factor for coherent excitation of the waveguide modes is higher.

The second way to enhance the coherence of the beam on the sample is by decreasing the sample size to a value equal to or below the vertical coherence length in the focus, which is given by the outermost zone width $d$ (see Fig. 4.4).
Now, the number of photons on the sample decreases with the sample size, but the flux gain caused by the introduction of the lens remains unchanged. In Fig. 4.12 the measured intensity distribution $I_1(\theta_1, \theta_e)$ is shown for a waveguide with a small gap and with a pre-focused beam. The upper surface was slightly tilted, such that the entrance gap $W_1 = 238$ nm and the exit gap $W_2 = 191$ nm. The waveguide at the entrance is now of the order of the local coherence length $\xi_{L,r}$. Except for the flux enhancement, the plot is similar to the plot without lens (not shown here), with only excited modes on the diagonal $\theta_e = \theta_i$. The condition for excitation of single modes, $\Delta \Omega < \Delta \theta$, can be rewritten using $\Delta \Omega = D/f$, which gives $W < d/2$, half the coherence length of the focused beam at the waveguide entrance. Therefore, the observation that single modes are excited in the presence of the lens is a good indication that the beam is coherent. Note though, that this argumentation is not valid when inverted. Excitation of multiple modes does not necessarily mean that the beam is incoherent.

4.6 Conclusions

We have demonstrated the use of a one-dimensional Fresnel-zone-plate lens for focusing a hard-x-ray beam onto the entrance of a planar x-ray waveguide. The achieved flux enhancement by a factor of 54 makes it possible to perform for example x-ray photon correlation spectroscopy studies of the dynamical properties of confined fluids. The propagation of a partially coherent focused beam through a waveguide can be described adequately by classical wave optics, as described in section 4.3 and appendix A. The approximation of the FZP lens by an ideal lens with a low-intensity plane-wave background proves to be sufficient to explain the observed diffraction patterns.

If a spatially coherent beam is required, one has to ascertain that the coherence is not destroyed by the lens on the length scales of the sample. A trade-off has to be made between flux enhancement and preservation of coherence. As demonstrated above, the coherence length can be tuned in two ways. We can adjust the aperture of the lens such that the coherence length at the sample is larger than the sample itself. However, by reducing the lens aperture, the flux gain is reduced. The focusing properties of the lens are more fully employed, with conservation of coherence, if the sample is made smaller than the coherence length in the focus. This is, however, not always possible and depends on the specific experimental conditions.

In the case that coherence is not required and just flux enhancement is desired, the lens diameter can be enlarged so that more flux is captured in the lens aperture. To keep the same demagnification factor, however, one then needs a smaller
outermost zone width, which may be beyond the limit of what is technically possible.

The observed effective source size with the lens and the waveguide inserted is twice the size observed without these two optical components. Seemingly, the coherence of the beam is affected by defects and roughness of these two components. We have demonstrated, however, that coherent propagation of waveguide modes in the waveguide is possible with a pre-focused beam.

So far, we have paid no attention to the fact that the lens affects the angular resolution of diffraction experiments in which the scattering vector is along the vertical focusing direction. If the convergence angle $\Delta \Omega$ of the incident beam is larger than the angular mode spacing $\Delta \theta$ and the modes are excited incoherently, the angular resolution is given by the angle $\Delta \Omega$, and thus the angular resolution is reduced. For coherent excitation of the modes, it should, in principle, be possible to deconvolve the convergence angle from the diffraction data, but this significantly complicates the analysis. If one investigates the in-plane (the non-focusing direction) structure or dynamics, this disadvantage is of course absent.