CHARACTERISATION OF X-RAY NANO-FOCUSING OPTICS WITH A GRATING INTERFEROMETER

The master thesis work summarized in this report has been realised as part of the Swedish civilingenjör degree
by Claude SANZ
in 2013-2014
The fabrication of X-ray nano-focusing systems is very delicate, which is why the quality of the wavefront after focusing is important information in order to determine the optics quality. Nowadays several tests are used to characterise nano-focusing optics, in this report two of them will be investigated in detail: the Ronchi test and a single grid array interferometer. The first one will give images analysed by comparison with a simulation, whereas the second one will give images that can be analysed using a Hartmann method and a method based on Fourier transforms. Two types of X-ray optics are investigated, a compound refractive lens and a zone plate. The results are that the compound refractive lens mainly affects the wavefront with a phase error localised around the optical axis, whereas the zone plates principally introduces coma and astigmatism to the wavefront. The conclusion of this report is two-fold: on the one hand the method based on Fourier transforms is quantitative and possible to use with single grid array interferometer results, whereas the Hartmann analysis is not suitable in this case. On the other hand, the Ronchi method is applicable to the hard X-ray nano-focusing alignment and delivers qualitative information about both the main aberrations introduced by the optics and the coherence of the setup.
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1 Introduction

X-rays are electromagnetic waves oscillating with a wavelength in the range of 0.01 nm to 10 nm. Such short wavelengths help increasing the resolution. It also means that the beam carries a lot of energy and can penetrate into material deeper than visible light. These are the reasons why it is possible to analyse many materials using X-rays, which makes the technique very interesting. However, X-rays are hard to produce due to high energy requirements. Nowadays, with the development of new technologies leading to powerful X-ray sources such as synchrotron facilities and X-ray free electron lasers, research based on X-rays is expanding. Especially growing are applications which use X-rays focused to nanometer-sized spots with X-ray optics. These nano-focusing optics are delicate to produce, which is why characterising methods are needed to evaluate their quality. There are currently many methods to analyse X-ray optics, such as grating interferometry [1] [2] [3], speckle tracking [4], pencil beam deflectometry [5], coherent diffraction imaging [6], and Hartmann wavefront sensing [7].

In this master thesis two different experiments are described, referred to as the Ronchi test and the single grid array interferometer. These experiments are realised with two types of focusing systems, namely one zone plate and one compound refractive lens. They will lead to two types of experimental data which will be analysed using three different methods: Ronchi simulation, Hartmann analysis and Fourier transform analysis. Note that the nano-focusing optics, the gratings, the data, the analysis methods performed and the conclusions presented in this report are results of a team work performed by Jussi Rahomäki, Daniel Nilsson, Ulrich Vogt, Fredrik Uhlén and myself, with the collaboration of Linda Lundström, Ulrich Wagner and Frank Seiboth, and that the experiments were accomplished at the coherence branch of I13 beamline at DIAMOND Light Source [8].

After an introduction to nano-focusing optics and grating interferometers in the second chapter, the working principle, the experimental arrangement and the analysis will be detailed for Ronchi images and single grid array interferometer successively in the third and fourth chapter. This will be followed by the conclusion of the master thesis work.
2 BACKGROUND

2.1 X-ray nano-focusing optics
In this chapter information about the nano-focusing systems is given.

In order to focus X-rays several types of optics exist: the ones based on reflection like mirrors which gather the beam in the two directions one after the other, or capillaries and waveguides which guide the X-rays from a source point to a focal point; the ones based on diffraction like multilayer mirrors, bent crystals and Fresnel zone plates; and finally the compound refractive lens based on refraction. This report focuses on the two last. Compound refractive lenses (CRL) are made of several lenses aligned to each other. Each of them makes a contribution by bending the rays of light which finally gather at the focal point [9]. They are commonly made of aluminium or beryllium, depending on the energy of the X-rays used in the experiment. Secondly there are zones plates (ZP), made of a substrate with a modulated layer of phase shifting material. The phase of the light is modified by the zone plate according to Fresnel’s distribution so that the X-rays also gather at a focal point [10]. The zone plates investigated in this thesis are made by Fredrik Uhlén: three different layers are spread onto a diamond substrate, a pattern corresponding to the zone plate is realised by electron-beam lithography on the first layer and transferred to the tungsten via several steps of reactive ion etching [11]. This fabrication process is the same for the gratings which are used as X-rays interferometers, described in the next paragraph.

2.2 X-ray grating interferometer
The analysis methods described throughout this report are based on an X-ray grating interferometer, the basic principle of which is explained in this paragraph.

The principle of X-ray grating interferometers is to create interferences using gratings to deduce the deformations of the wavefront caused by the focusing system. There are different ways of realising this: it can be done using several gratings with different periods aligned with each other, straight [1] [2] or tilted [3]. In the two experiments presented in this thesis, the interferences are created by only one grating. They result from the intersection between the different orders of diffraction of the grating. For the Ronchi image the interferences are resulting from two orders, whereas the single grid array interferometer is the result of the superposition of many orders. It is due to the fact that the periods of the grating differ by one order of magnitude. As smaller periods lead to a larger angle between the different orders, they become either superposed to each other or separated on the resulting image at the detector plane. As a result, the interferences composing the Ronchi images are spread on a bigger area, so that higher partial coherence is required to obtain an image, which gives information on the coherence of the alignment. On the other hand, the single grid array interferometer has the advantage that only one image is required, carrying all the information. More details about the grating interferometer leading to the Ronchi images are given in the next chapter, as well as the results obtained.
3 THE RONCHI EXPERIMENT

The experimental setup corresponding to this testing method is simple. As shown in Figure 1, a grating, positioned close to the focal plane, splits the light beam in different directions corresponding to different orders of diffraction. Two of the created light beams interfere with each other, which create a Ronchi pattern on the detector. This pattern contains information about the wavefront. The analysis consists of comparing the measured patterns with simulated ones in order to deduce the aberrations in the beam.

![Diagram of the Ronchi experiment]

3.1 Working principle

In this chapter the theory, upon which the Ronchi experiment is based, is described in detail.

3.1.1 Properties of the grating

The Ronchi experiment is based on the proper use of a grating as a beam splitter [12]. Different useful properties of the optics in this experiment are described in this paragraph.

To optimise the visibility of the Ronchi image we need to share the incident intensity $I_0$ so that we see the orders of diffraction $k=-1$, $k=0$ and $k=+1$ with similar intensity for the energy used in the experiment. These orders of diffraction appear with negligible to high intensity $I$ when we change the phase shift $\varphi$ between two consecutive stripes. When we modify this phase shift, the grey curve displayed in Figure 2 happens to slide along the x-axis, so that it changes the intensity of the orders of diffraction from zero to four times the intensity after an absorption grating. In Figure 2 (a-d) the results from different phase shifts $\varphi$ are displayed, from which we deduce the best choice for our application.
Characterisation of X-ray nano-focusing optics with a grating interferometer

(a) Intensity repartition after a $2\pi$-shift grating

(b) Intensity repartition after a $\pi$-shift grating

(c) Intensity repartition after a $\pi/2$-shift grating

(d) Intensity repartition after a $0.64\pi$-shift grating

---

Figure 2: Intensity repartition after different kinds of phase shift gratings

The best choice for the phase shift is a $0.64\pi$-shift grating. Nevertheless, it is very hard to create gratings with periods as small as the one used for the Ronchi test, namely about 200 nm, with a thick layer of tungsten. This is the reason why in the experiment with the 8.5 keV X-rays, a $\pi/2$-shift grating is used, which gives a sufficient contrast in the resulting Ronchi images to analyse the data. After this adjustment is done, another important parameter is the overlap of these visible orders of diffraction in order to obtain the highest possible visibility.

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The Ronchi image results from the overlap of the orders of diffraction $k = 0$ and $k = \pm 1$. As can be seen from the simulation results in Figure 3, the overlap of the images from these different orders must be so that the discs from orders $\pm 1$ have a tangent in the middle of the disc of order 0. In this configuration, the part which carries information is extended as much as possible. To do so, we have to choose the right grating period. As a consequence, it is good to think about arranging several
gratings with different periods. Finally, what we are going to see in this experiment as soon as the gratings are well adjusted will be detailed in the next chapter: the Ronchi image.

### 3.1.2 Ronchi image

The Ronchi image is the result of interferences between the different orders of diffraction of the grating. It carries information about the optical quality of the focusing alignment such as the type of main aberrations and the coherence of the source. To analyse it we need to simulate it, as described in this paragraph.

The simulation of the Ronchi image is straightforward. First, an aberrated surface is generated in the exit pupil of the optical system to simulate the wavefront after its propagation through the optical system. Secondly, this surface is transferred numerically along the optical axis to the grating, using the Fourier method (detailed in [13], chapter 11.3.3). The grating is simulated by an additional phase following a grid shape. After the grating, diffraction occurs while the surface is propagated towards the detector plane. Finally, we extract the interference pattern to make the Ronchi image appear on the detector plane. This image is the result of the superposition of different typical patterns linked to the aberrations. Indeed, there is a definite interference pattern, which can be described by a mathematical function, corresponding to each type of aberration [14]. Through the images displayed in Appendix 1, we will discover some of the patterns, namely the ones corresponding to the predominant aberrations we have observed in the focusing systems we measured (which will be introduced in a following chapter). Furthermore, the Ronchi image gives information about the coherence of the optical alignment through the contrast of the fringes. Indeed, without sufficient coherence the contrast of the fringes would drop. This is why one can use the Ronchi method to determine if the optical configuration is suitable for an experiment. The different experimental values of the elements used in the Ronchi test are described in the following chapter.

### 3.2 Experimental arrangement

The Ronchi test and the single grid array interferometer test are using almost the same experimental arrangement, only the distances between the focal point and the grid array and the grating period change.

The first sample is a compound refractive lens composed by 30 lenses made of beryllium, each with a radius at the apex of the parabola of 50 µm, giving a theoretical focal length of 179 mm. The exit pupil is limited by a 300 µm diameter hole in order to obtain as high partial coherence as possible for the ptychography experiment which was led by Frank Seiboth [15]. In practice the aperture is about 250 µm due to the absorption by the beryllium at 8.5 keV. Note that in order to prevent the creation of beryllium oxide during the experiment due to X-ray absorption leading to heating of the lenses, they are confined in a box with a helium atmosphere. The second and third sample are a 75 µm diameter zone plate with an outermost zone width of 50 nm, whose quality has already been evaluated during a previous experiment [11], and a 500 µm diameter zone plate with an outermost zone width of 100 nm, on which we will focus in this report. This latter zone plate has a focal length of 334 mm. The cross which is visible in the measurements is due to the addition of an external 100 µm diameter central stop. The aim of the central stop is to protect the camera from the non-deviated light coming from the source, corresponding to the 0-order of the zone plate.
The detector is a 150 μm thick CdWO4 scintillator, imaged by a 5x magnification microscope objective on a Manta camera with 6.45 μm x 6.45 μm pixel size. As the final goal of the experiment is to have an easy-to-realize way of characterising the nano-focusing elements for X-ray light in any synchrotron, it is logical to show that the technique works on this common type of detector. The images we obtain have a high number of pixels per fringes, which makes the analysis easy and accurate. Additionally an ion chamber is used as an intensity controller.

In order to create interferences, we need sufficient spatial and temporal coherence. Particularly in the Ronchi experiment, the coherence must be high enough to make interferences possible on the whole aperture. The experiment in the DIAMOND light source took place about 180 meters away from the source, and the source could be limited by a slit to assure high spatial coherence. The high temporal coherence is assured by the monochromator which delivers an 8.5 keV X-ray beam. If we do not have enough coherence in one direction, the contrast of the interferences in this direction will drop. A drop of the contrast can also be due to an inaccurate choice of the grating period, which in this experiment is either 200 nm, or 210 nm. These periods allow the Ronchi image to appear on the detector which is 18 cm away from the focal point while shifting the grating through the focal area about a few millimetres along the light axis. The Ronchi images obtained from this experimental setup are presented and analysed in the next chapter.

3.3 Results and analysis
The analysis of the Ronchi data is done by comparison between the measured data and some modelled data which are adjusted to fit the measurements. In this chapter, in the Figure 4 to 8 you can see the results obtained for horizontal and vertical grating stripes, firstly for the compound refractive lens and secondly for the zone plate. The results from the Ronchi analysis are deduced from the images and given in the Tables 1 to 4.

3.3.1 Compound refractive lens (CRL); horizontal stripes, 210 nm period

![Figure 4: Ronchi images obtained with a compound refractive lens from a scan through focus](image-url)
Claude SANZ

The Ronchi experiment

<table>
<thead>
<tr>
<th>Nature of the information at the exit pupil</th>
<th>Amount (W/λ; grating’s period)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Astigmatism</strong></td>
<td></td>
</tr>
<tr>
<td>vertical</td>
<td>present but faint</td>
</tr>
<tr>
<td>oblique</td>
<td>absent</td>
</tr>
<tr>
<td><strong>Coma</strong></td>
<td></td>
</tr>
<tr>
<td>vertical</td>
<td>absent</td>
</tr>
<tr>
<td>oblique</td>
<td>absent</td>
</tr>
<tr>
<td><strong>Spherical</strong></td>
<td></td>
</tr>
<tr>
<td>vertical</td>
<td>present</td>
</tr>
<tr>
<td>horizontal</td>
<td>absent</td>
</tr>
<tr>
<td><strong>Grating’s shift</strong></td>
<td></td>
</tr>
<tr>
<td>vertical</td>
<td>present</td>
</tr>
<tr>
<td>horizontal</td>
<td>present but faint</td>
</tr>
</tbody>
</table>

Table 1: Analysis for CRL; grating with horizontal stripes, 210 nm period

3.3.2 Compound refractive lens (CRL); vertical stripes, 200 nm period
When the first measurements with vertical stripes were done in the synchrotron laboratory, there was no interference in the image on the detector. We deduced from this result that there was not enough horizontal coherence. After different trials it appeared that the disruptive element was the water-cooling of the monochromator. The results in Figure 5 have been taken after we stopped the cooling system.

![Ronchi images](image1)

**Table 2:** Analysis for CRL; grating with vertical stripes, 200 nm period
3.3.3 Zone plate (ZP); grating with vertical stripes, 200nm period

Figure 6: Ronchi images obtained with a zone plate from a scan through focus

<table>
<thead>
<tr>
<th>Nature of the information at the exit pupil</th>
<th>Amount (W/λ; grating’s period)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Astigmatism</td>
<td></td>
</tr>
<tr>
<td>vertical</td>
<td>present</td>
</tr>
<tr>
<td>oblique</td>
<td>present</td>
</tr>
<tr>
<td>Coma</td>
<td></td>
</tr>
<tr>
<td>vertical</td>
<td>absent</td>
</tr>
<tr>
<td>horizontal</td>
<td>present and predominant</td>
</tr>
<tr>
<td>Spherical</td>
<td>absent</td>
</tr>
<tr>
<td>Grating's shift</td>
<td></td>
</tr>
<tr>
<td>vertical</td>
<td>–</td>
</tr>
<tr>
<td>horizontal</td>
<td>present</td>
</tr>
</tbody>
</table>

Table 3: Analysis for ZP; grating with vertical stripes, 200 nm period
3.3.4 Zone plate (ZP); horizontal stripes, 200nm period

![Ronchi images obtained with a zone plate from a scan through focus](image)

Figure 7: Ronchi images obtained with a zone plate from a scan through focus

<table>
<thead>
<tr>
<th>Nature of the information at the exit pupil</th>
<th>Amount (W/λ; grating’s period)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Astigmatism</td>
<td></td>
</tr>
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<td>vertical</td>
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<tr>
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<tr>
<td>Grating’s shift</td>
<td></td>
</tr>
<tr>
<td>vertical</td>
<td>–</td>
</tr>
<tr>
<td>horizontal</td>
<td>present</td>
</tr>
</tbody>
</table>

Table 5: Analysis for ZP; grating with horizontal stripes, 200 nm period

3.4 Conclusion of the Ronchi experiment analysis

The use of the grating determines the quality of the Ronchi image. To obtain a well visible image fitting with a real grating, the grating’s phase shift has been chosen as π/2. The overlap of the images can be adjusted by choosing a proper grating period. With only little experience of the Ronchi method it is possible to quickly get information about the coherence of the optical arrangement and predominant aberrations of the optical focusing system.

The focusing systems which are evaluated in the experiments are a compound refractive lens (CRL) with a focal length $f_{CRL} = 179\text{mm}$, and a zone plate (ZP) with a focal length $f_{ZP} = 334\text{mm}$. The grating used for the Ronchi test have 200 nm and 210 nm periods, with either vertical or horizontal stripes. The detector is 18 cm away from the focal point.
From the clearness of the images in Figure 4 we can determine that there is high partial vertical coherence and from Figure 5 that there is less partial horizontal one. From the analysis summarised in Table 1 and 2 we conclude that the main aberration introduced by the CRL is well fitted with spherical aberration. We also conclude from the changes in the grating shift that the translation is not stable in both x and y directions. The zone plate is larger than the compound refractive lens as it has an 500µm diameter, which leads to a drop of contrast due to the decline in coherence on the whole aperture, and implies faint Ronchi images. The conclusion from Tables 3 and 4 is that the main aberrations of the zone plates are coma and astigmatism.

The Ronchi experiment was already performed with an X-ray free electron laser source and gave satisfying results [16]. The aim of doing it again is to prove that it is possible to perform it with a synchrotron light source and that it is a valid method to quickly verify the quality of an optical alignment: its coherence and its main aberrations, although it is not a quantitative method but more a qualitative one. It is possible to obtain quantitative results with other configuration and analysis methods, like the one presented in next chapter.
4 THE SINGLE GRID ARRAY INTERFEROMETER

The experiment we will refer to as the single grid array interferometer test uses quite a similar setup to the Ronchi test, as shown in Figure 8. Indeed, the experiment is realised with larger gratings, further away from the focal plane. In this configuration it is no longer the Ronchi pattern which is observed, but the first Lohmann image of the grating, also resulting from interferences. In this image there is a grid of dots whose positions depend on the aberrations introduced by the optical system. The Hartmann analysis, based on the comparison between the measured grid and a reference grid, as well as another analysis method based on Fourier transform will be discussed in this chapter.

4.1 Working principle
4.1.1 Talbot effect and first Lohmann image

The Talbot effect explains why the image of the grid is observable on the detector, whereas the first Lohmann image is the result of the configuration used in this experiment.

The experiment alignment comprises a phase shifting grating which uses a grid pattern. If the illumination is sufficiently coherent, a near field diffraction effect occurs, which is called Talbot effect. Talbot discovered the fact that the light emerging from an absorbing grating recreates the grating’s pattern at definite distances called Talbot distances. On the other hand, when the light emerges from a periodical phase-object with a fitting phase shift, it creates an intensity pattern at definite distances which are fractions of the Talbot distance. When the contrast of this pattern is 100%, the corresponding image is called a Lohmann image [17]. Whereas the period of the grating have been computed previously by Daniel Nilsson, we dealt with the problem of which phase shift to use. As the fabrication of a thin phase shift is easier to obtain, we chose the smallest phase shift for
which we have data about the Lohmann image, which leads to a π/2-shift grating. We also decided to work with the first Lohmann image in this experiment, the closest to the grating. This image is interesting as we can measure its intensity with a photo-detector.

4.1.2 The Hartmann method
The Hartmann method is one of the methods used to analyse the data from this experiment. It is based on the comparison of the position of the measured dots with the position of the dots of a reference grid.

Thanks to the Talbot effect, an image of the grating is obtained on the detector. This image is not a perfect image of the grating, as the light used to create it has been focused by a non-perfect optical element. These imperfections will slightly shift the luminous parts of the grating, by Δx and Δy. These deviations can be measured relative to the reference grid: a perfect grid with the same width and number of dots as the measured image. It gives information about the wavefront W as a function of the distance d between the grid and the detector:

\[
\frac{\partial W}{\partial x} = \frac{\Delta x}{d} \quad \text{&} \quad \frac{\partial W}{\partial y} = \frac{\Delta y}{d}
\]  
(4.1)

The Hartmann analysis consists of fitting all the small deviations between the reference grid dot positions and the real dot positions by the Zernike polynomials

\[ Z_j(x, y) = Z_n^m (x, y) \quad \text{with} \quad j = \frac{n(n + 2) + m}{2} \]  
(4.2)

From the polynomial coefficients obtained by this step it is possible to recompose the wavefront and then display it as

\[ W(x; y) = \sum_{j=0}^{j_{\text{max}}} W_j Z_j(x, y) \quad \text{with} \quad W_j = W_n^m \]  
(4.3)

Note that we said previously that the precision of the Hartmann analysis method is linked to the number of illuminated dots. Indeed we can consider each dot as a data point in the wavefront reconstruction. Remember also that when the wavefront is obtained, it can be propagated so that we know the distribution of the light at all positions in our system, particularly at the focal point [19]. Another method used to analysis the same type of image is based on Fourier transforms.

4.1.3 The Fourier transform method [20]
The Fourier-transform method is the second method used to deduce the optical quality of the focusing system from the data.

The Fourier transform method got its name as it is based on the manipulation of data contained in the Fourier space, as illustrated by Figure 9. Indeed, if a grid can be described using complex numbers as

\[ g(x, y) = a(x, y) + c(x, y) e^{2\pi i f_0 x} + c^*(x, y) e^{2\pi i f_0 x} \]

with \( c(x, y) = \frac{b(x,y)}{2} e^{i\phi(x,y)} \)  
(4.4)
the first step is to apply a discrete Fourier transform with the respect of $x$ to the whole aperture of the grid of dots to obtain

$$G(f_x, f_y) = A(f_x, f_y) + C(f_x - f_0, f_y) + C^*(f_x + f_0, f_y)$$

In the 2D Fourier space, we find the spatial phase variations in the two perpendicular directions $\Phi_x$ and $\Phi_y$, which are contained in two particular dots corresponding to the horizontal and vertical grating’s first orders. These dots can then be isolated and shifted to the centre of the Fourier space as the spatial variations of $a(x, y)$, $b(x, y)$ and $\Phi(x, y)$ are slow compared to the variations of $f_0$. Then an inverse Fourier transform gives $c(x, y)$, that is to say a partial wavefront. The two wavefronts corresponding to the two directions $x$ and $y$ are then combined [21] so that we obtain the final result: the aberrated wavefront resulting from the experimental setup, introduced in the next paragraphs.

**Figure 9: The different steps for the Fourier transform analysis**

<table>
<thead>
<tr>
<th>a) Crop of the image</th>
<th>b) 2D Fourier transform</th>
<th>c) Isolation + centering</th>
</tr>
</thead>
<tbody>
<tr>
<td>d) Combination of the two perpendicular partial wavefronts</td>
<td></td>
<td></td>
</tr>
<tr>
<td>e) Wavefront</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### 4.2 Experimental arrangement, results and analysis

Once the position of the grating has been chosen, the grid of dots is obtained on the detector, as you can see in Appendix 3. The experimental arrangement followed by the different results obtained from the single grid array interferometer data, either using the Hartmann method or using the Fourier transform method are described and discussed in this paragraph.

The experimental arrangement is quite the same as the one described for the Ronchi experiment (Chapter 3.2), only now the grating is placed 3 cm from the focal point and the period of the grid is 2 $\mu$m. Although the image is a result from interferences, medium partial coherence is enough as the distance between the images resulting from the different orders of diffraction of the grating are very close to each other.

The result is that the Hartmann analysis method cannot be applied to the type of data obtained with the single grid array interferometer test as the position of the reference grid is not possible to
determine without being relative to the measured grid, which implies inaccurate results. Due to the absence of information in the centre of the grid while measuring a zone plate, it is not possible to apply the Fourier transform method to the single grid array interferometer image resulting from a zone plate. So the information obtained from the Fourier transform method is the wavefront resulting from a compound refractive lens (CRL), which is presented in this image:

![Figure 10: Results from the Fourier transform method for a CRL](image)

4.3 Conclusion of the single array interferometer analysis
The conditions of the experiment are very similar to the Ronchi ones. However, the grating is a π/2-shift grating with a 2 µm period grid pattern, placed about 3 cm away from the focal point: at the position of the first Lohmann image.

The Fourier transform method is an effective method to characterize the type of data obtained with the single grid array interferometer, while the Hartmann analysis proves to be inaccurate. The advantage of the Fourier transform analysis is that it only one single image. The result obtained with this method is an aberration located in the centre of the lens, which may be due to the fabrication process of the compound refractive lenses.
5 Conclusion

The master thesis work presented in this report is about the analysis of the results collected at the coherence branch of the I13 beamline at the DIAMOND light source with a 8.5 keV X-ray beam. Two different experimental setups led to Ronchi images and single grid array images. They have been analysed following three different methods: Ronchi simulation, Hartmann analysis and Fourier transform analysis; in order to characterise two different kinds of X-ray nano-focusing optics: a compound refractive lens and a zone plate.

On the one hand, the Ronchi analysis is a qualitative analysis, which delivers information on the main aberrations present in the alignment and the coherence of the beam; it can be used as well to verify or improve the alignment of the focusing system by reducing the field aberrations, which are astigmatism and coma. The Ronchi method works for the zone plate as well as for the compound refractive lens.

On the other hand, the Hartmann analysis is not accurate enough to be applied on the single grid array interferometer results, while the Fourier transform analysis is a method which is appropriate for the compound refractive lens. Nevertheless, its application to the zone plates with the grid patterns without the central part will require further research to be reliable. This method gives quantitative information on the aberrations present in the measured nano-focusing system, and only requires one single image from the alignment to be applied, without the need for high partial coherence.

To conclude, the aberrations introduced by the compound refractive lens are specific to this type of focusing system. It is not spherical aberration which is found, but a pattern coming from a non-perfect hyperbolic shape in the beryllium lenses. The aberrations introduced by zone plates are coma and astigmatism. Furthermore, two useful methods can be applied to get relevant information about X-ray nano-focusing systems and the alignment from one or a few images, namely the Ronchi and the Fourier transform analysis.
Appendix 1  
SIMULATED RONCHI PATTERNS

The following images show simulation results with an amount of aberration of $\lambda/2$ at the exit pupil of the focusing system. The first row is simulated with a grating with vertical stripes whereas the second row is simulated with a grating with horizontal stripes.

Note that for spherical aberration it exists different foci (paraxial and marginal), here the images ‘at focus’ are taken from the area with fewer fringes.

---

a. Pure defocus, no aberration

b. Spherical aberration
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c. Vertical coma

1mm before focus
At focus
1mm after focus

Vertical coma

1mm before focus
At focus
1mm after focus

d. Horizontal coma

1mm before focus
At focus
1mm after focus

Horizontal coma

0.5mm before vertical focus
At vertical focus
1mm after vertical focus

Vertical astigmatism

1mm before horizontal focus
At horizontal focus
0.5mm after horizontal focus

1mm before focus

At focus

f. Oblique astigmatism

1mm after focus
Appendix 2  SIMULATION AS AN ANALYSIS TOOL

The modelled data is created by the user through an interface. This simulation interface needed to be as thorough and accurate as possible, as well as convenient for the user. Indeed, at first the interface was very simple: as you can see in Appendix 2.1, there only were entries for the amount of aberrations, which would then be expressed with the Seidel coefficients; and entries for the different elements required for the computation of the field and the generation of the Ronchi image. The graphs showed the wavefront created, the absolute value of the field at the grating plane and the simulated Ronchi image. In order to improve its usefulness for the experimental setup in DIAMOND, some changes have been made. As you can see in Appendix 2.2, entries have been added for the characteristics of the detector, so that the simulated image (after being resized) looks like it should appear on the detector, in a new graph. The names of the entries have been changed to appear clearer to the user. A button “determine grating’s position for the first Lohmann image” has been added, so that either the user can enter the distance himself, or he can enter the characteristics of the alignment and get the position by pressing the button. Also, as the focusing systems were of two kinds, namely a Zone Plate ZP and Compound Refracting Lens CRL, a window has been added so that after choosing the kind of focusing system we can enter the characteristics which are treated differently in the MATLAB script. Particularly the precision of the computed focal length of the CRL has been increased. An important feature is also that the size of the grey total window is fixed and needed to be small enough to fit on the screen of a laptop to be brought in the experiment environment.
Appendix 2.1  Before modifications (Realized by Daniel Nilsson)

This is the original interface realized by Daniel Nilsson during his PhD work [22].
Appendix 2.2 When ready for the experiment

For the Single grid array interferometer experiment we only brought the MATLAB code to the lab which gave us the position of the first Lohmann image when we entered the distance from the focus to the grating. This script has been written following this reasoning: we remember from 4.1.1 that we decided to work with the Lohmann image the closest to the grating in order to have more data points. As we work with a π/2-shift grating, the distance to the first Lohmann image \( R_L \) is one quarter of the Talbot distance \( R_T \) [17] (first line of table 1, p.4689), and it can be expressed in terms of the grating period \( d \) and the wavelength \( \lambda \) as

\[
R_L = \frac{R_T}{4} = \frac{d^2}{2\lambda} \tag{A-1}
\]

Nonetheless this is given for a grating illuminated by a plane wave, yet we work in a diverging wave which changes the distance \( R_L \) so that we can express it with the distances \( R_1 \) from the focal point to the grating and \( R_2 \) from the grating to the detector (see Figure 8) as follows:

\[
R_L = \frac{R_1 R_2}{R_1 + R_2} \tag{A-2}
\]

We finally want the closest position of the grating for a given focal point position and a given detector position, so that after introducing the quantity \( R_{\text{tot}} = (R_1 + R_2) \) we solve the equation

\[
R_L = \frac{R_1 R_{\text{tot}} - R_1^2}{R_{\text{tot}}} \Rightarrow R_1^2 - R_{\text{tot}}R_1 + R_L R_{\text{tot}} = 0
\]

and we obtain

\[
R_1 = \min \left( \frac{-R_{\text{tot}} - \sqrt{R_{\text{tot}}^2 - 4R_L R_{\text{tot}}}}{2}; \frac{-R_{\text{tot}} + \sqrt{R_{\text{tot}}^2 - 4R_L R_{\text{tot}}}}{2} \right) \tag{A-3}
\]

This equation was added to the script used by the interface so that the slide position was adjusted when the button was pressed.

For the Ronchi analysis the important elements were the grating period needed in order to obtain the right overlap and the size of the cells of the detector in order to prevent being limited by the pixelation. This is why the first change realised on the interface was to add a graphic with a pixelated image according to the size of the detector pixels (realised by resizing the image with the right amount of pixels). To get the right size for the final image we needed to change the focal length equation which was not precise enough, so instead of using the focal length introduced by the user, we asked the user for the different characteristics of the compound refractive lens (\( \delta \) the refractive index decrement of the material, \( \beta \) the absorption coefficient, \( l \) the length of one lens, \( R \) the radius at the apex of the parabola, \( N \) the number of lenses) and compute from this information the focal length according to [23]:

\[
f = \frac{1}{\sqrt{\frac{2\delta}{\Gamma \ast R} \sin \left(N \ast l \ast \sqrt{\frac{2\delta}{\Gamma \ast R}} \right)}} \tag{A-4}
\]
Note that this equation uses the refractive index decrement $\delta$ which we needed to obtain previously. For this we needed to create a look-up table for different energies and the two most probable materials, namely aluminium Al and beryllium Be. Finally, to predict the appearance of the measured image the Gaussian absorption function resulting from the shape of the compound refractive lens (CRL) [24] was added. It is function of the coordinates $x$ and $y$ of the ray going through the lens and $d$ the thickness in the centre of one lens constituting the CRL, as well as function of the wave number $k$, in addition to the parameters found in (A-5), as

$$T = e^{-k(\beta-i\delta)\left(\frac{N(x^2+y^2)}{k}+d\right)} \quad \text{(A-5)}$$

With these accurate details we knew what to expect as results and after minor adjustments of the size of the aperture, we obtained similar results from the model and the measurements. At this point we could comprehend directly what we saw and get the data for a future deeper analysis.
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Appendix 2.3 Ready for the analysis

In order to perform the analysis some more modifications have been realised. Indeed, from the experiments which were performed well thanks to the predictions of the model, we obtained much Ronchi data. This data consists of images taken as the grating was translated through the focal point. The interest of having a scan through the focal point is that we obtain the evolution of the fringes with the defocus, which makes the identification of the aberrations of the focusing system more accurate. To pinpoint the aberrations of the compound refractive lens, we decided to compare the measurements with modelled data. In order to simplify the comparison, the interface has been modified: the theoretical image on the detector plane has been replaced by the measured image corresponding to the amount of defocus entered by the user. Indeed, the displayed image changes according to the amount of defocus indicated so that it corresponds to the modelled image, if the limit values of the defocus slide are well adjusted. This way it is possible to adjust the amount of aberration so that the model fits one image, and to move along the light direction so that the model fits the best all the different images.
Appendix 3

EVOLUTION OF THE HARTMANN IMAGES FOR INCREASING Z

$z = z_0$

$z = z_0 + 1\text{mm}$

$z = z_0 + 2\text{mm}$

$z = z_0 + 3\text{mm}$

$z = z_0 + 4\text{mm}$
First of all, I want to thank Ulrich V. for inviting me to join the group and accepting to be my supervisor; for the confidence he has placed in me for the duration of my master thesis, for his time and his support, as well as his very helpful answers to my questions and his understanding.

Then I want to thank Hans, for having accepted to be my examiner, making the realisation of this master thesis possible, as well as for his support and his understanding.

I thank Daniel, Jussi, Fredrick and Linda for their time and answers, their work to help me and for the energy they gave me when I needed some, as well as all of BioX group for their welcoming atmosphere and their support; DIAMOND light source and Ulrich W. for the beam time and the technician assistance, Franck for the compound refractive lens and the help during the experiment.

I thank Jussi, Birte, Thomas, Fredrick, Daan and Ulrich V. for proof reading.

I would have liked to thank my late father who believed in my success until the end, giving me the strength to finish this work despite my sorrow. I wish to thank my mother and grandparents, who understood all my choices and supported me throughout my studies.

I would also like to thank all of my friends and particularly Daan, Birte, Ludovic, João, Adrien, Armande, Maude, Julie, Fabienne and my siblings François and Nicolas, for their patience regarding my English, their friendship and their support throughout my studies.
REFERENCES


