2D grating simulation for X-ray phase-contrast and dark-field imaging with a Talbot interferometer

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Abstract. Talbot interferometry is a recently developed and an extremely powerful X-ray phase-contrast imaging technique. Besides giving access to ultra-high sensitivity differential phase contrast images, it also provides the dark field image, which is a map of the scattering power of the sample. In this paper we investigate the potentialities of an improved version of the interferometer, in which two dimensional gratings are used instead of standard line grids. This approach allows to overcome the difficulties that might be encountered in the images produced by a one dimensional interferometer. Among these limitations there are the phase wrapping and quantitative phase retrieval problems and the directionality of the differential phase and dark-field signals. The feasibility of the 2D Talbot interferometer has been studied with a numerical simulation on the performances of its optical components under different circumstances. The gratings can be obtained either by an *ad hoc* fabrication of the 2D structures or by a superposition of two perpendicular linear grids. Through this simulation it has been possible to find the best parameters for a practical implementation of the 2D Talbot interferometer.

Keywords: X-ray phase-contrast imaging, X-ray dark-field imaging, grating interferometry, Talbot effect, Fresnel propagation

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INTRODUCTION

X-ray imaging is a unique tool for non-destructive inspection of bulky materials; it finds successful applications in various fields such as medical and biological imaging, non-destructive testing, materials science, geoscience, paleontology, homeland security and many other fields. Conventional transmission radiography and tomography are based on the signal originated from the imaginary part of the complex refractive index while the information given by the real part of it is usually not accessible.

Although for many applications this is not a problem, it imposes severe limitations when low density objects or details with small absorption difference with respect to the surrounding material need to be imaged. This is the case, for example, of soft tissue imaging in biomedical specimens.

These limitations can be overcome with phase-contrast imaging techniques: they convert the phase shift induced by the sample into intensity modulation and use this information as the main (or unique) source for the image formation [1]. In the past decades various X-ray phase contrast methods have been developed and studied. Among these are free space propagation [2] [3] [4], analyzer based imaging [5] and crystal interferometry [6] [7].

They have all extensively shown that phase contrast imaging can yield information not accessible to absorption radiography but they require high spatial and/or longitudinal coherence, high stability and/or complicated

set-ups. This is why their usage is usually limited to synchrotron radiation facilities or micro-focus X-rays tubes, the latter with low flux, and they have not been widely exported outside the research laboratories.

A new technique called grating (or Talbot) interferometry has less stringent requirements, and has shown excellent results since its first development in 2002 [8] [9]. The set-up has several advantages: it is simple and compact, it has been demonstrated to work also with conventional X-ray tubes [10] [11] [12] and gives access to large field of view and high sensitivity phase images, see for example [13].

This paper contains a brief review of the working principle of the standard X-ray Talbot interferometer and the image processing procedure usually performed. This introduction is followed by a discussion on the problems that might be encountered in a standard experiment, in which line gratings are used.

The approach studied in this work consists in a two dimensional (2D) grating interferometer which can overcome the difficulties of the standard method. The feasibility of the method and the best parameters for a practical implementation of it are illustrated in the final part of the paper. The central part of the paper is dedicated to an explanation of the simulation methods.

X-RAY IMAGING WITH A 1D GRATING INTERFEROMETER

The detailed principles of Talbot interferometry are described in [14] [15]. The experimental set-up of a standard Talbot interferometer is shown in Fig 1.

FIGURE 1. Scheme of a conventional X-ray Talbot interferometer set-up.

The optical elements are two high aspect ratio linear gratings [16] [17] positioned between the sample and the detector; their lines are oriented perpendicular to the optical axis and one parallel to the other. The first grating G1 encountered by the X-rays is a beam splitter which provides a periodic modulation to the phase of the incident wavefront and, preferably, negligible absorption. At a distance corresponding to a fractional Talbot order [18] [19] from this, the phase modulation is transformed into an intensity fringe pattern through the Talbot effect [20]. The distances at which the self-imaging phenomenon occurs are the working points for an X-ray interferometer. For an incident plane wave, they are dependent on the wavelength λ of the X-rays and the period p of G1 by the formula [11]:

$$D = n \frac{p^2}{2\lambda\eta^2} \quad \begin{cases} \eta = 1 & \pi/2 \text{ shifting grating} \\ \eta = 2 & \pi \text{ shifting grating} \end{cases} \quad (1)$$

where n is an odd number.

If an object is placed in the beam path, the interference fringes are locally shifted and reduced in amplitude as schematically shown in Fig. 2.

The goal of X-ray grating interferometry is to detect the wavefront distortions induced by the specimen. The image detector alone is usually not sufficient for this purpose because the pixel size is similar to or larger than the fringe period. An amplitude grating G2, with the same periodicity as the intensity pattern, is therefore used as an analyzer element. It is placed immediately before the image sensor with the absorption lines parallel

FIGURE 2. A sample in the X-ray path induces distortions in the interference fringes formed through the Talbot effect. The analyzer grating serves to resolve the interference pattern. The phase stepping technique is used to quantify the effect of the specimen on the incident wavefront. A quantitative analysis of the property of attenuation, scattering and phase-shifting of the object is thus possible.

to the interference fringes. The phase stepping technique, well established in visible-light interferometry [21], is used to separate the phase information from the other contributions to the signal: one of the two gratings is scanned along the x direction over a few fringe periods. In the following, let m be the number of fringe periods over which the phase stepping scan is performed (usually 1 or 2), and l the number of steps in the scan (at least 4 per period).

Three different image modalities

Ideally, the intensity oscillation measured in each image pixel should be a triangular function because it is given by the convolution of two box profiles: the fringe profile created by G1 and the transmission profile of G2. Due to the imperfections in the optical elements together with the partial coherence of the radiation, it is often more similar to a sinusoidal curve (Fig. 3).

Three different and complementary types of image signals can be extracted by analyzing the intensity variation in each pixel. This is usually done by considering the 0-th and m -th orders of the Fourier transform of the values measured in each detector pixels during the phase stepping scan, under the assumption that higher orders can be neglected.

1. The conventional *absorption* image, as if the interferometer were not in the beam, can be obtained by taking the average value of the intensity measured during the phase stepping scan. This corresponds to A_0 , the 0-th order Fourier component.
2. The phase of the intensity oscillation, after the reference beam subtraction, is related to the angular deflection α_x of the X-rays by the object in the di-

FIGURE 3. Intensity oscillation observed during a phase stepping scan with $l = 32$ steps over $m = 1$ one period. The intensity values are given in arbitrary units. The phase, amplitude and mean value of the intensity sinusoidal curve are extracted with the Fourier analysis.

rection perpendicular to the grating lines. Since α_x is given by

$$\alpha_x = \frac{\lambda}{2\pi} \frac{\partial \Phi}{\partial x}$$

[22], the phase of the intensity oscillation is proportional to the *differential phase shift* ($\partial \Phi / \partial x$) induced by the specimen along the x direction. This corresponds to ϕ_m , the phase of the m -th Fourier component. A quantitative measure of the phase shift caused by the object, can be obtained by a one dimensional integration along the image lines.

3. The incoherent scattering of the sample reduces the amplitude of the interference fringes. A measure of the loss in visibility due to the presence of the specimen is therefore related to the scattering power of the object. This gives the so-called *dark field* image which essentially reveals the microscopic density fluctuations in the sample [23]. This corresponds to A_m/A_0 , twice the modulus of the m -th Fourier component normalized by the 0-th component.

2D GRATING INTERFEROMETER

Motivations

The one dimensionality of the optical elements and the directional information that they provide may lead to different problems, especially in the phase and dark-field images.

- The strength of the differential phase and dark-field signals depends on the orientation of the details in the specimen. The maximum signal is obtained for details oriented parallel to the grating lines y , on the other hand any feature oriented along the x

direction is not revealed in these two types of image modalities.

- The one dimensional integration of the differential phase image is done by assuming the boundary condition that the initial phase shift is zero. This constraint is not valid if the object is larger than the field of view; in this case a quantitative phase analysis is not possible.
- When samples details have too strong phase gradients, the phase information is lost due to the phase wrapping effect which causes artifacts similar to those produced by noise. A second source of phase image noise is the poor count statistics which impedes the determination of the phase in the phase stepping scan curve.
- A new type of image signal has recently been exploited; it gives the directional dark-field image which essentially reveals the orientation inside the specimen of the scattering structures. Until now this can only be obtained by recording radiographies at different angular positions of the sample around the optical axis.

These problems can be overcome by simultaneously accessing the information along two perpendicular directions in the image plane: x and y [24].

This paper presents numerical simulations describing the optical configuration for a two dimensional (2D) grating interferometer. This device, already introduced in [25] [26], is used to retrieve and combine the dark-field and differential phase signals along two orthogonal axis. The phase grating is a 2D structure with phase shifting pillars, it induces a 2D periodical intensity pattern at particular distances. The analyzer grating must also be a bi-dimensional grid. The phase stepping scan of one of the two optical elements is performed in two dimensions.

Simulation methods

The Talbot effect with 2D gratings has been simulated for the case of a coherent unit-amplitude plane wave illumination. The optical elements are modeled with their complex transmission function in the thin-object approximation. The Fresnel propagation of the wavefront along the optical axis is calculated in Fourier space under the paraxial approximation [27].

By following the evolution of the intensity distribution along the beam path it is possible to find the optimal configuration for 2D X-ray grating interferometry imaging. The desired intensity distribution is a binary periodic pattern in the x and y directions.

The gratings that have been considered have the same periodicity p along x and y and the width of the grating

structures equal to the spacing between them.

They are assumed to be ideally phase shifting (giving either π or $\pi/2$ phase shift) and non-absorbing structures. The performances of a checkerboard-type (CB) phase grating with an area duty cycle of 0.5, (Fig 4) have been compared to those of a mesh-type (M) grid with an area duty cycle of 0.25, Fig. 5. The simulation of the phase stepping scan is done by a 2D convolution of the phase grid image with an analyzer grating consisting of opaque structures.

FIGURE 4. Checkerboard (CB) type of 2 dimensional grating. The active parts are in white, the area duty cycle is 0.5.

FIGURE 5. Mesh (M) type of 2 dimensional grating. The active parts are in white, the area duty cycle is 0.25.

RESULTS

Table 1 summarizes the results of the simulation of different G1 types (first column). The distances at which self-images of the grating appear are listed in the second column of the Table in terms of n , that has to be substituted in Eq. 1. The images produced by the gratings and their periodicity are illustrated in Fig. 6 and reported in the last two columns of the Tab. 1.

TABLE 1. Results of the simulation of different types of 2D phase gratings (first column), Fig.6. The distances at which binary intensity patterns are formed are given in the second column in terms of n that has to be substituted in Eq. 1. In the first line of the Table, k is an integer non-negative number $k = 0, 1, 2, 3, \dots$. The grating images and periodicities are reported in the last two columns respectively and shown in Fig. 6.

G1 type	Phase shift	Distances n in Eq. 1	Image type	Period
M	π	$n = 4 + 8k$	CB	p
M	$\pi/2$	$n = 1.5, 3.5, 5.5, \dots$	M'	p
CB	π	$n = 1, 3, 5, \dots$	M	$p/2$
CB	$\pi/2$	$n = 0.5, 1.5, 2.5, \dots$	CB	p

The results summarized in Table 1 are shown in Fig. 6 (a) – (d).

(a) Mesh π – shifting grating:

(b) Mesh $\pi/2$ – shifting grating:

(c) Checkerboard π – shifting grating:

(d) Checkerboard $\pi/2$ – shifting grating:

FIGURE 6. Left, phase modulation induced by the phase grating [rad]; right relative intensity [a.u.] at the observation plane.

The M type π -shifting and the CB type $\pi/2$ -shifting gratings produce a CB intensity pattern with the same periodicity as G1; a ‘negative’ self-image is created by a mesh grid with $\pi/2$ -shifting pillars.

The images produced by a π -shifting CB type grating are mesh intensity patterns with half of the periodicity of the grating itself. This 2D structure is the most suitable for a practical implementation of the 2D Talbot interferometer for the following reasons:

- The π -shifting CB is the only structure among the ones in Tab. 1 that can be created by the simple superposition of 2 orthogonally oriented linear phase shifting gratings. The lines of the two gratings are perpendicular with respect to the optical axis. Fig. 7 shows that, in the overlapping regions, the total phase shift is $2\pi = 0$ resulting in a $0 - \pi$ checkerboard pattern.

FIGURE 7. Top. The superposition of two linear π -shifting gratings, one perpendicular with respect to the other, results in to a 2D checkerboard grating with π -shifting pillars. In the overlapping region the total phase shift is $\pi + \pi = 2\pi = 0$. Bottom. The superposition of two ideal opaque linear gratings one perpendicular to the other yields a 2D mesh absorption grating. In the overlapping region the transmission is 0%.

- The n values at which the mesh images appear are the same as in the 1D case (odd values). They are much denser distributed along the optical axis with

respect to the M type π -shifting structure, giving a wider choice of grating distances.

- The halving of the periodicity allows the usage of larger G1 structures, easier to fabricate, for a desired fringe period at the detector plane. The smaller the period, the better the spatial resolution.

In analogy to the phase stepping scan of the 1D case Fig. 3, the intensity distribution of the wavefront at the observation plane is determined by the scanning of one grating in two directions. The two dimensional phase stepping scan corresponds to a sampling of the 2D convolution of the interference pattern with the transmission function of the analyzer grid. In the following let us denote the convolution operation by the ‘*’ symbol. The simulated analyzer gratings have the same periodicity as the intensity pattern and ideally 0% transmitting structures. Since there are two different bi-dimensional patterns, there are four possible convolution combinations which reduce at three due to the symmetric property of the convolution operation. They are:

1. CB intensity pattern * CB analyzer grating
2. CB intensity pattern * M analyzer grating =
M intensity pattern * CB analyzer grating
3. M intensity pattern * M analyzer grating

FIGURE 8. Left. Image resultant from the 2D convolution of a CB intensity pattern with a CB analyzer grating (case 1.) or from the convolution of a mesh and checkerboard patterns (case 2.). Right. Image produced by the 2D convolution of a mesh intensity pattern with a mesh analyzer grating (case 3.). They represent the image that is sampled during a phase stepping scan. They have been calculated over 4 periods.

Fig. 8 left shows the results from cases 1. and 2. in the above list; the convolution of 2 mesh patterns (case 3.) gives the image (Fig. 8 right). The latter pattern is preferred if the phase stepping scan is analyzed with the 2D Fourier analysis which can also provide the information along the diagonals. Note that a mesh type absorption grating can be realized with the superposition of two independent linear absorbing structures, one rotated by 90 degrees with respect to the other (Fig. 7 bottom).

The most suitable 2D grating interferometer is given by the combination of a checkerboard π shifting grating and a mesh absorption grid which has half of the periodicity of the phase grating. They can both be obtained by

the superposition of two linear structures, rotated by 90 degrees one respect to the other. Fig. 9 shows this type of 2D grating device essentially consisting of two orthogonal standard Talbot interferometers. The working distances D are the same as the 1D case, they correspond to the fractional Talbot orders.

FIGURE 9. Scheme of a 2D Talbot grating interferometer.

CONCLUSIONS

The uni-directional information of the standard 1D X-ray Talbot interferometer leads to limitations which can be overcome with the usage of a 2D system.

A numerical study on different types of 2D gratings has allowed to find the optimal configuration for a 2D grating interferometer. The simulation has been carried out using Fresnel propagation in the paraxial approximation and the optical elements are described with their complex transmission function.

The binary intensity image produced by different types of gratings has been evaluated and the 2D phase stepping scans have been simulated. It has been found that the preferred configuration is given by a π -shifting checkerboard grating in combination with a mesh type absorption grid with half the periodicity of the phase grating.

A 2D grating interferometer following this principle can be implemented either with *ad hoc* fabricated 2D gratings or with the combination of two independent 1D interferometers rotated by 90 degrees one respect to the other. The working distances of the 2D grating interferometer are the same as the 1D version. The mesh image produced by G1 is analyzed via a 2D phase stepping scan by moving one of the two optical elements on a mesh grid in the plane perpendicular to the optical axis. The intensity distribution measured during the scan can be analyzed with the 2D Fourier transform. The information coming from the two orthogonal directions can be combined to improve the dark-field and phase images quality

and overcome the limitations intrinsically present in the 1D case.

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