Propagation-based x-ray phase contrast imaging using an iterative phase diversity technique

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Abstract
Through the use of a phase diversity technique, we demonstrate a near-field in-line x-ray phase contrast algorithm that provides improved object reconstruction when compared to our previous iterative methods for a homogeneous sample. Like our previous methods, the new technique uses the sample refractive index distribution during the reconstruction process. The technique complements existing monochromatic and polychromatic methods and is useful in situations where experimental phase contrast data is affected by noise.

Keywords: x-ray, Fresnel region, imaging, near-field, iterative, phase contrast

((Some figures may appear in colour only in the online journal)

1. Introduction

We have previously shown that an iterative reconstruction applied to propagation-based near-field x-ray phase contrast data can have a wider range of applicability than analytical techniques [1], such as the contrast transfer function [2, 3] and transport of intensity equation [4].

The iterative technique is capable of recovering the complex transmission function of the sample—meaning quantitative determination of the sample’s thickness distribution is possible—under both monochromatic [1] and polychromatic [5] illumination.

However, we have also shown [1] that loss of information in the recorded phase contrast image—for example, due to noise or source blur—has the potential to introduce artefacts—such as a cross-hatching effect—into the iterative reconstruction, thus impacting the quality of the reconstructed object image.

A potential solution to this problem can be found through the use of phase diversity techniques. These methods were originally explored to find common elements in multiple images which contained noise or suffered other aberrations in incoherent imaging systems [6]. The benefits of phase diversity can be introduced through a number of different methods including implementing additional planes of detection [7], employing different focus distances [8], varying the longitudinal and transverse position of the probe on the sample [9] and using multiple energies [10–13].

In this work, we show that a multiple wavelength phase diversity technique combined with a near-field phase contrast iterative technique is capable of recovering thickness information with fewer artefacts for homogeneous objects [14]. This new phase diverse method significantly reduces the...
cross-hatching artefact that was encountered in our mono-
chronic iterative algorithm [1].

2. Algorithm

Since the thickness of the object is independent of wave-
length, it can be used to ensure consistency between mea-
surements taken at each wavelength. The algorithm is similar
for an individual wavelength used in [5] and shown here in
equations (1)–(6). The incorporation of multiple wavelengths
through the consistency of the thickness is managed as shown
in equations (7) and (8). The calculated sample thickness, \( t \), is

\[
t_j = \left( \frac{\ln (T_{j})}{-k_j (\beta_j + i \delta_j)} \right),
\]

(1)

where the subscripts here and in the following equations refer
to the \( j \)th wavelength, \( \lambda \), used in the measurement, \( k \) is
the wavenumber, \( k = \frac{2\pi}{\lambda} \), and \( \beta \) and \( 1 - \delta \) are the absorption
and phase components of the complex refractive index. The
transmission function is given by

\[
T_{j} = \frac{\psi_{0,j}}{\psi_{j}},
\]

(2)

where \( \psi_{0,j} \) is the incident wavefield.

Following the operator notation often used in CDI
[15–17], successive iterations to the wavefield, \( \psi \), can be obtained using

\[
\psi^{j+1} = \pi_m \psi^j \psi_{j}.
\]

(3)

The support constraint is

\[
\pi_m \psi_{j} = \begin{cases} 
\psi_{j} & r \in S \\
\psi_{0,j} & r \notin S,
\end{cases}
\]

(4)

where \( S \) defines the region of support that contains the sample
and \( r \) is the position vector within the wavefield. The modulus
constraint is defined by

\[
\pi_m = P^{-1} P_m P,
\]

(5)

where \( P \) and \( P^{-1} \) are the forward and reverse propagation
operators respectively and

\[
\pi_m \psi_{j} = \frac{\psi_{j}}{|\psi_{j}|} |T_{j}|,
\]

(6)

where \( I \) is the measured intensity and \( \psi \) is the detector plane
wavefield.

Here, we use the Fresnel propagator in its convolution
form [19] to propagate between the sample and detector
planes. The iterative algorithm is a solution for the lack of
phase information recorded at the detector and in our imple-
mentation the initial wavefield is initiated using a random
value for the phase of the wavefield.

With multiple wavelengths at each iteration we can apply
equations (1) and (2) to obtain estimates for the thickness.

Then using the inverse of equations (1) and (2) with the next
wavelength values, the current estimate for the next wavefield
is produced, which can then, in turn, be used in equation (3).
This operation can be represented by \( \pi_m \) as

\[
\psi^{j+1} = \pi_m \psi^{j} = \exp[-t_j k_{\lambda_j} (\beta_{\lambda_j} + i \delta_{\lambda_j})] \psi_{0,j}.
\]

(7)

We can represent the overall phase diversity process by

\[
\psi^{j+1} = \prod_{j=0}^{M-1} (\pi_m \pi_{\lambda_j} \pi_{\lambda_j}) \psi^{j}.
\]

(8)

where \( \Pi \) represents the successive application of the opera-
tions and \( \pi_{\lambda_{j-1}} \) sets the energy back to \( \lambda_0 \).

An alternative approach could be to use the average
estimate for the thickness obtained from each wavelength to
generate the next iterate for the wavefield.

Convergence of the algorithm can be monitored by
comparing a \( \chi^2 \) difference between the current and previous
estimate for the diffracted intensity for any of the measured
wavelengths used [1].

Any energy of interest can be used to monitor the
convergence of the algorithm at the detector plane. A more
robust convergence metric can also be applied by requiring
that \( \chi^2 \) fall below a pre-set threshold for all wavelengths used.

Convergence of the reconstructed thickness estimate, \( t_n \),
can also be monitored for simulation test cases by comparing
a \( \chi^2 \) difference between the current estimate for the thickness
with the known value [1].

The benefits of the phase diverse method compared to single
and polychromatic wavelength reconstructions are demonstrated
in figure 1. In this example, the test object used in the exper-
imental demonstration was simulated under conditions that
demonstrate artefacts in the reconstruction. A Gaussian source
blur of 2 \( \mu \) full width half maximum (FWHM) with a random
signal to noise ratio of 3% was applied to the simulated phase
contrast image for the test object, which has thickness of 350,
650 and 1000 nm in the regions as shown in figure 1(a). The
image was oversampled on a 710 \( \times \) 710 array. The source to
distance, \( z_1 \), and sample to detector distance, \( z_2 \), were
0.76 m and 0.24 m, respectively. The pixel size at the detector
was 450 nm. Figures 1(b) and (c) show the monochromatic
reconstructions for \( \lambda = 0.138 \) nm (9 keV), \( \delta = 2.67 \times 10^5 \)
and \( \beta = 2.31 \times 10^6 \) and \( \lambda = 0.0954 \) nm (13 keV), \( \delta = 1.24 \times 10^5 \)
and \( \beta = 1.51 \times 10^6 \), respectively, (d) shows a polychromatic
recovery using a 9–13 keV spectrum in bins of 100 eV, while (e)
is the phase diverse reconstruction. Although we have used
wavelength notation above, we will refer to the corresponding
energies for experimental convenience below. The phase diverse
reconstruction provides a better-quality image, significantly
reducing the cross-hatching artefact seen in the monochromatic
and polychromatic reconstructions. It can also be seen in
figure 1(f) that the phase diverse method converges faster than
either the monochromatic or the polychromatic simulations.
Table 1 shows the standard deviation of the recovered thickness
divided by the mean of the recovered thickness—a percentage
thickness error—for each of the reconstruction methods. Near
the sharp edges of the object, the sampling assumptions used in
the propagation and in the analytical formula are invalid due to the sudden change in wavefield’s phase at these points [3]. Accordingly, the regions indicated in figure 1(a) are used to assess the recovered thickness. While the average values recovered over the regions are similar, the percentage thickness error for the phase diverse method is less than the percentage thickness error for either the monochromatic or polychromatic reconstructions.

3. Experiment

An experimental demonstration of the algorithm was undertaken using Diamond Light Source’s B16 Test Beamline [18]. A conventional in-line phase imaging geometry was employed. Phase diversity was achieved by acquiring phase contrast images at two distinct energies—9 and 13 keV.

For both energies, a point source with a vertical and horizontal FWHM of 0.607 and 0.837 μm respectively was created using a Kirkpatrick–Baez mirror. z₁ and z₂ were 0.76 m and 0.24 m, respectively.

Twenty phase contrast and flat-field images were acquired at each energy, all with an exposure time of 75 s. The detector employed was a cooled 14 bit charge-coupled device camera coupled with a YAG:Ce 35 μm thick scintillator and 20× objective lens.

The sample used for the experiment is shown in figure 2(a). It was made from two overlapping patterns of Au deposited on a Si₃N₄ window. The thickness was 350, 650 and 1000 nm in the blue, green and red regions indicated respectively.
Figure 2. Experimental demonstration. (a) Schematic of the Au sample used for experimental demonstration. Reproduced from [1]. © 2016 IOP Publishing Ltd and Deutsche Physikalische Gesellschaft. CC BY 3.0. (b), (c) The single and twenty image averaged phase contrast images for 9 keV, respectively. (d) The regions that were used to calculate the mean thickness in table 2. The test regions have a nominal thickness 1000 nm (red), 650 nm (green) and 350 nm (blue). (e), (f) The single and twenty image averaged phase contrast images for 13 keV respectively. (g), (h) The single image reconstructions for 9 and 13 keV. (i) The single image reconstruction for the phase diverse method using 9 and 13 keV. (j), (k) The twenty-image reconstruction for the phase diverse method using 9 and 13 keV, respectively. (l) The twenty-image reconstruction for the phase diverse method using 9 and 13 keV.
4. Analysis

The experimental measurements were used to create two datasets for each energy. The first dataset used all of the 20 experimental measurements of the phase contrast and flat-field images. The second dataset only used the last phase contrast measurement acquired and first flat-field measurement acquired (i.e. the phase contrast and flat-field measurements that were closest in time). The phase contrast images for both the 9 and 13 keV datasets were divided through by the relevant flat-field images to remove variations in the illumination and scintillator non-uniformity. Despite the flat-fielding of the datasets, the background in the phase contrast was still not perfectly uniform due to time variations in the illuminating beam. The resultant images can be seen in figures 2(b), (c), (e) and (f).

One thousand iterations of our monochromatic iterative algorithm [1] were applied to each of the four datasets using a loose support. Propagation between the sample and detector plane was completed using the Fresnel propagator in its convolution form [19]. The detector \( \chi^2 \) was used to monitor the convergence of the algorithm for each of the datasets. The thickness reconstruction for these monochromatic sets can be seen in figures 2(g), (h), (j) and (k).

The phase diverse algorithm was applied to the 9 and 13 keV phase contrast images to reconstruct the sample thickness for both the single and twenty image datasets. For both datasets, 1000 iterations were applied using the phase diverse algorithm and a loose support. The Fresnel propagator in its convolution form was again used to propagate between the sample and detector planes. A \( \chi^2 \) test as described in the algorithm section was used to monitor the convergence of the algorithm for each of the datasets. The thickness reconstruction for the phase diverse method can be seen in figures 2(i) and (l).

The time variability in the illuminating beam meant that the phase contrast images were not uniform. Accordingly, the reconstructions of the object were also not uniform over large spatial regions, even where the regions are known to be of uniform thickness. This is particularly evident in the lower left part of the reconstruction shown in figure 2(j). The fact that the non-uniformity is more pronounced in this image, which was from 20 repeat exposures, then it is in figure 2(j), which is from a single exposure, is a clear indicator that the variation between exposures does not average out to a uniform result.

Fortunately, the effect that we are seeking to demonstrate here is that phase diversity can ameliorate the loss of information in the phase contrast image that results in higher spatial frequency artefacts, such as the cross-hatching shown in simulation and experimentally in figures 2(g), (i), (j) and (k). This can be verified by measuring the uniformity of the recovered object over a smaller region than used in the simulations described in the algorithm section. The regions used in each of the different thicknesses of the object are shown in figure 2(d).

The resulting measured percentage thickness error for each of these regions is shown in table 2. While we have not compared the experimental results for the regions shown in figure 2(d) with those obtained using our polychromatic approach [5], the percentage thickness error obtained in [5] was 10% or greater for each thickness but for a larger bandwidth, which improved the results. Accordingly, while a similar error is expected in the smaller regions as for the larger regions due to the uniform reconstruction obtained in that experiment, it is not expected to be any better than the 10% result previously obtained. Therefore, the experimental results are consistent with simulations described in the algorithm section. It can be seen overall that the phase diverse method gives a lower percentage thickness error in each case, consistent with the visual impression of greater uniformity of the phase diverse method given in figure 2.

5. Conclusion

The phase diverse method presented in this paper adds an additional tool for those attempting to undertake reconstructions in the near-field. We have shown the phase diverse technique significantly reduces the cross-hatching artefact that can be encountered with our previous monochromatic iterative algorithm. The approach could also be generalised to measurements taken with multiple polychromatic illumination conditions.

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