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Influence of finite spatial coherence on ptychographic reconstruction

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X-ray ptychography is an ultrahigh-resolution scanning coherent diffractive imaging technique, allowing quantitative measurements of extended samples and a simultaneous reconstruction of the illuminating wavefront. Recent development of the mixed-state reconstruction algorithm has triggered a certain interest in utilizing partially coherent X-ray sources for ptychography. Here, we study how finite spatial coherence influences the reconstructed image of a test structure. Our work shows that use of a highly coherent illumination provides images with better spatial resolution and fewer artefacts than the approach with partial coherence. © 2015 AIP Publishing LLC.

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The low-emittance third-generation synchrotron light sources and advances in instrumentation¹ have extended the use of X-ray microscopy to nanoscale-objects. Lens-based phase contrast imaging has broadened the hard X-ray metrology to even weakly absorbing biological specimens.^{2–4} Moreover, with the development of lensless imaging methods, limitations of X-ray optics could be circumvented using numerical methods for solving the phase problem.^{5,6} Ptychography^{7,8} is a high-resolution scanning coherent diffractive imaging (CDI) technique. It measures multiple far-field diffraction patterns from partially overlapping areas.⁹ The overlap is then used by iterative phase retrieval algorithms^{10–12} as a constraint to recover both the sample object and the illumination function (probe). The retrieved object function represents the quantitative optical density of an investigated sample.¹³ Ptychography offers spatial resolutions restrained only by the numerical aperture of the detector and the finite amount of measured photons in high scattering angles. Recently, ptychographic imaging with 10-nm spatial resolutions has been demonstrated for strongly scattering test samples in the hard X-ray regime.^{14,15} Conventional ptychographic reconstruction relies on a high degree of coherence. Yet, radiation produced by an undulator source at synchrotron facilities is only partially spatial coherent. Utilizing only coherent flux decreases the available intensity of diffracted radiation, limiting measurement speed, resolution, and image quality. Alternatively, the mixed-state ptychographic reconstruction¹⁶ can deal with partially coherent illumination, demanding though larger datasets for successful convergence.

In this letter, we studied the influence of finite spatial coherence on ptychographic reconstruction. We performed ptychographic measurements on a strongly scattering Siemens star test object in different coherence conditions. Spatial resolutions of images obtained with conventional (single-mode) and mixed-state algorithms were compared. We report also the achievable resolving power of the utilized scanning

X-ray microscope using 2D ptychographic imaging with highly coherent illumination.

Experiments were performed at beamline P11 at the PETRA III synchrotron light source at DESY in Hamburg. The beamline is dedicated to high-resolution X-ray imaging and diffraction experiments.¹⁷ P11 optics are equipped with two horizontally and one vertically deflecting X-ray mirrors ready to operate in concave (focussing) and flat bending modes. Both horizontally deflecting mirrors can additionally be bent convexly, defocusing the X-ray beam and hence increasing horizontal spatial coherence. Ptychographic imaging was carried out using the experimental setup as shown in Fig. 1. The coherent portion of a beam was selected with an off-axis beam defining pinhole (BDP) that illuminated a Fresnel zone plate (FZP). Calculated theoretical transverse coherence lengths¹⁸ in the BDP plane equalled $21 \times 129 \mu\text{m}^2$ ($h \times v$) at an energy of 6.4 keV. The first order focus was selected by an order sorting aperture (OSA). The direct beam was blocked by a central stop (CS). The sample was placed slightly downstream of the back-focal plane to provide an illumination size of about 1 μm . This was set by tuning faintly the energy, while keeping the FZP-sample distance fixed. Using a computer-controlled piezomotorized x/y stage, the sample was scanned perpendicularly to the beam. Regular grid-scan positions were randomly offset up to 50% of the step size to avoid raster-grid pathology.¹¹ The far-field diffraction patterns were recorded with a single photon counting Pilatus 1M pixel detector.¹⁹ Along the propagation distance, an evacuated flight tube was installed to suppress absorption and scattering of X-rays in air. Ptychographic reconstructions were performed using two difference-map-based²⁰ algorithms: (1) conventional, assuming fully coherent single-mode illumination,¹¹ and (2) mixed-state, allowing partially coherent X-rays.¹⁶

In the first experiment, we studied how finite spatial coherence influences ptychographic reconstruction. To achieve that, two off-axis BDPs of different diameters were used in the experimental setup as in Fig. 1. The test sample was a 700-nm-thick Siemens star with the smallest spoke size of 50 nm, manufactured by electron beam lithography and gold

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FIG. 1. Scheme of the ptychographic experimental setup using an off-axis illuminated zone plate and a single photon counting Pilatus 1M pixel detector.

electroplating.²¹ Ptychographic scans of the Au-Siemens star were recorded using off-axis BDPs of diameters: 20 μm and 50 μm , and the entirely illuminated 100- μm -diameter FZP. In the latter two cases, aperture size exceeded the horizontal transverse coherence length. Detailed parameters of the experimental setup are summarized in Table I (Experiment I).

Reconstructed phase shift images obtained with the conventional algorithm are shown in Fig. 2. In insets, the reconstructed amplitudes are presented. For further analysis, the reconstructed phase shift images were chosen as they provided a better contrast and were less prone to artefacts than the reconstructed amplitudes.

At the highest spatial coherence conditions (Fig. 2(a)), all spokes of the Au-Siemens star are clearly resolved. The larger the diameter of the off-axis BDP (Figs. 2(b) and 2(c)), the more pronounced artefacts become, causing substantial loss of information. In Fig. 2(c) (entirely illuminated FZP), the pattern is severely distorted. The edges of the vertical spokes are additionally much worse resolved than those of horizontal spokes, which stems from the different transverse coherence lengths in these both directions.

Subsequently, as shown in Fig. 2(a), at each spoke, between the second and the third ring of the Au-Siemens star (marked with red dashed arcs), several line profiles of a spoke's edge were extracted, as marked with blue and orange lines.²² To each line profile, an error function was fitted and an average of obtained full-width at half-maximum (FWHM) values for a given spoke's edge was taken. The

average vertical or horizontal FWHM components were then corrected for an inclination angle θ with an appropriate trigonometric function, yielding the total average FWHM (FWHM_{tot}). Such analysis allowed to obtain the angular dependences of the FWHM_{tot} for the reconstructed phase images for different illumination schemes (Fig. 3). As expected, the best spatial resolution (about 30 nm) occurs in conditions of the highest degree of spatial coherence (20 μm off-axis pinhole) and remains constant within one pixel at all inclination angles. A moderately decreased degree of coherence (50 μm off-axis pinhole) worsens the resolution (larger FWHM_{tot}) up to about 45 nm. Finally, illumination of an entire zone plate with partially coherent beam (100- μm -diameter FZP) results in a significant deterioration of resolution. An angular dependence of FWHM_{tot} is clearly noticeable in this case. Edge profiles from horizontal spokes (at smaller angles) are better resolved than the edge profiles from vertical spokes (those at larger angles). This proves the significant difference between the vertical and the horizontal transverse coherence lengths. Error bars²³ are considerably large in the case of 100- μm -diameter FZP (up to 30%) due to severely distorted Siemens star edges' profiles. In Table II, the FWHM_{tot} at the extreme θ values (3° and 93°) are summarized for all illumination schemes, showing the average vertical and horizontal spatial resolutions.

The same datasets were then reconstructed using mixed-state algorithm. Only three probe modes were retrieved, as intensity fractions of further modes were less than 2% of the total probe intensity,^{16,24} yielding no further improvement of spatial resolution. Figs. 4(a) and 4(b) show 3-mode ptychographic reconstructions of the Au-Siemens star images for measurements with 20 μm and 50 μm off-axis BDP. For these cases, intensity fractions in the orthogonalized probe modes are listed in Table III. In the case of 100- μm -diameter FZP, neither of the higher modes converged. The retrieved object image was the same as in the conventional reconstruction and hence is not presented. Fig. 4(c) compares the $\text{FWHM}_{\text{tot}}(\theta)$ dependences between corresponding conventional (Figs. 2(a) and 2(b)) and 3-mode (Figs. 4(a) and 4(b)) phase shift reconstructions. The 3-mode reconstruction approach applied to the low-degree-of-coherence image (50 μm pinhole) corrects for decoherence artefacts, yet, does not make FWHM_{tot} reach the high-degree-of-coherence case (20 μm pinhole). It may be partly due to a slight increase of horizontal spatial coherence in the latter case caused by convex bending of one horizontally deflecting mirror.

In the second experiment, we determined the achievable resolving power of the utilized scanning X-ray microscope.

TABLE I. Detailed parameters of two experiments.

Parameter	Experiment I ^a	Experiment II
Energy (keV)	6.4, <u>6.4</u> , 6.56	6.2
BDP (diameter) (μm)	20, 50, –	20
CS (diameter) (μm)	–, <u>30</u> , 30	–
FZP (diameter) (μm)	100	100
FZP (outermost zone) (nm)	100	60
OSA (diameter) (μm)	10	10
Propagation distance (m)	4.04	4.40
Exposure time (s)	1	1
Horiz. probe size ^b (μm)	0.69, <u>1.60</u> , 0.78	0.45
Vert. probe size ^b (μm)	0.66, <u>1.52</u> , 0.91	0.49
Horiz. deflecting mirror 1	flat, flat, flat	convex
Horiz. deflecting mirror 2	convex, flat, flat	convex
Vertically deflecting mirror	flat	flat

^aDifferent illumination schemes: regular – 20 μm off-axis pinhole, underlined – 50 μm off-axis pinhole, **bold** – entirely illuminated FZP.

^bFull-width of half-maximum of a Gaussian fit.

FIG. 2. Conventional reconstructions of a complex object function of the Au-Siemens star using two off-axis BDP of following diameters: 20 μm (a) and 50 μm (b), and entirely illuminated FZP (c). Pixel size: 5.7 nm in (a) and (b) and 5.5 nm in (c), scan format: 61×61 scan points, and step size: 100 nm.

In order to compensate for the missing information in diffraction patterns at the intermodular gaps of Pilatus 1M detector, we performed a ptychographic measurement at two positions of the detector.¹⁴ This substantially diminished image artefacts.

Such modified ptychographic experiment was conducted to obtain images of a high-resolution nano-fabricated Siemens star made by coating a hydrogen silsesquioxane

FIG. 3. Evaluation of spatial resolution (FWHM_{tot}) for reconstructed phase images in Fig. 2. As shown in Fig. 2(a), several vertical and horizontal profiles (blue and orange lines, respectively) between the second and the third ring (red dashed arcs) were chosen to evaluate FWHM_{tot} , at different spokes' edges inclination angles θ .

template with a 10-nm-thick layer of Ir.²⁵ Again, an off-axis illumination of the FZP ensured selection of the coherent flux. Horizontal spatial coherence was improved by defocusing the X-ray beam with both horizontally deflecting mirrors (convex bending). Parameters of the experimental setup are listed in Table I (Experiment II). Reconstructed amplitude and phase shift images of the Ir-Siemens star's central part are presented in Fig. 5(a). Strong signals from 10-nm-thick Ir layers can be easily distinguished at all spokes' edges.

Quantification of spatial resolution limits of the images was performed by means of their averaged power spectral density (PSD) curves.²⁶ PSD-based analysis provides, namely, information on entire image in average and on all length scales, being therefore less subjective.

Fig. 5(b) presents the averaged PSD curves of the reconstructed amplitude (solid red line) and phase shift (dashed blue line) images of Ir-Siemens star. In both cases, the effective spatial resolution limit was determined by the intersection point (black arrows) of an averaged PSD curve and twice the level of featureless region dominated by noise.²⁷ The cut-off frequencies indicate therefore the half-period spatial resolution limits of the amplitude image at 10.1 nm and of the phase shift image at 10 nm, which are very close to the pixel size (8.3 nm).

In conclusion, our results show that ptychographic CDI utilizing highly coherent illumination provides reconstructed images with considerably better spatial resolution and fewer artefacts than the approach with partial coherence. Although mixed-state ptychographic reconstruction is an effective way to compensate for experimental imperfections, introducing additional modes requires recording proportionally more scan points (larger dataset) necessary for successful reconstruction. While the use of a partially coherent photon flux causes no significant gain in reconstructed information, it increases severely the dose which may be detrimental to

TABLE II. Summary of the FWHM_{tot} values at extreme angles of spokes' edges for all illumination schemes. Values in round brackets are the standard uncertainties.

Illumination scheme	FWHM_{tot} at $\theta = 3^\circ$ (nm)	FWHM_{tot} at $\theta = 93^\circ$ (nm)
20 μm off-axis pinhole	28.4(1.2)	35.81(0.43)
50 μm off-axis pinhole	48(12)	44.8(6.3)
100- μm -diameter FZP	71(22)	178(56)

FIG. 4. 3-mode reconstructions of a complex object function of the Au-Siemens star using off-axis BDP of diameters: 20 μm (a) and 50 μm (b). Pixel size: 5.7 nm. In (c), comparison of spatial resolutions ($\text{FWHM}_{\text{tot}}(\theta)$) between conventional and 3-mode phase shift reconstructions. Only for 50 μm pinhole, spatial resolution improves in the 3-mode case.

TABLE III. Intensity fractions in the orthogonalized probe modes obtained from 3-mode reconstructions.

Diameter of an off-axis pinhole (μm)	First mode (%)	Second mode (%)	Third mode (%)
20	91.0	6.0	3.0
50	67.5	23.7	8.8

FIG. 5. Conventionally reconstructed complex object function (a) of the Siemens star coated with 10 nm layer of Ir from the dataset recorded at two detector positions. Pixel size: 8.3 nm, scan format: 11×11 scan points, and step size: 100 nm. PSD analysis of the reconstructed amplitude and phase shift images in (b). Arrows indicate spatial resolution limits (half-period): 10.1 nm in the amplitude image and 10 nm in the phase shift image.

radiation sensitive samples. Furthermore, increasing the available flux with partially coherent illumination does not yield results superior to using highly coherent X-rays and conventional reconstruction algorithm. Therefore, with the latter approach, we demonstrated ptychographic imaging with a spatial resolution of 10 nm, performed at two detector positions. This all points towards diffraction-limited sources²⁸ able to provide the most coherent and intense synchrotron X-ray beam. Together with precise in-vacuum scanning X-ray microscopes and future seamless area detectors, they will certainly facilitate robust high-resolution ptychographic imaging.

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