Experimental comparison of full and partial coherent illumination in coherent diffraction imaging reconstructions

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Abstract: In this paper, we will present coherent diffraction imaging reconstruction of a well-known object by use of a Hybrid Input-Output algorithm. The sample was imaged at 400 nm wavelength with a fully coherent laser source and at 0.41 nm wavelength in partially coherent illumination. The comparison of the two experiments, completed with theoretical simulations, will highlight the influence of the degree of spatial coherence in the reconstruction process.

1. Introduction

Coherent Diffraction Imaging (CDI) is a powerful technique allowing for lensless imaging of any sample placed under coherent illumination. The technique uses the diffraction pattern observed in the far field to retrieve both amplitude and phase components of the object under test [1, 2]. Since no lens is used between the sample and the detection planes, the useful information is aberration-free and can be uniquely inverted to yield the electron density map of the sample. Several iterative algorithms [3, 4] have been developed for this purpose; the resolution of the recovered reconstruction being only limited by the experimental setup and the detector geometry.

In the hard X-ray regime, nanometer scale CDI of microscopic objects has become quite feasible. Nevertheless, the transverse coherence lengths obtained from 3rd and 4th generation sources (few tens of microns to only few microns at the sample position) prevent imaging over “large” fields of view. This is generally compensated by refocusing the X-ray beam before the sample and creating secondary sources to increase the degree of spatial coherence. Ptychography is also another alternative [5]. Furthermore, extended works on the influence of partial coherence in CDI have been done [6, 7], and phase retrieval algorithms, that take into account the illumination coherence function, enable strong enhancement of the reconstructions [8, 9].

In this paper, we propose to observe the influence of transverse coherence in the CDI reconstruction process, by using a well-known amplitude sample of finite size. After a brief discussion about our reconstruction algorithm and some experimental design considerations, we will present two experiments: the first one in the visible range with fully coherent illumination of the sample, the second one in the hard X-ray regime by using only partially coherent illumination. Analysis of the reconstructions in both cases, together with theoretical simulations, is used to validate our phase retrieval algorithm and to investigate partial coherence limitations in X-ray CDI experiments.

2. HIO algorithm principle
For sample reconstruction, we used a Hybrid Input-Output (HIO) [1, 10] algorithm, which is one of the most commonly used in CDI data treatment. This algorithm consists of iterative estimations of the sample (real space) from its observed diffraction pattern in the far field (reciprocal space).

First a random phase is assigned to the amplitude measured in the far field, and inverse Fourier transform of this complex function leads to the corresponding electromagnetic field in real space (Figure 1). From there, the algorithm relies on back and forth Fourier based calculations to estimate the electromagnetic field in real and reciprocal spaces successively. Convergence of the algorithm is forced by applying two constraints per iteration: a specific support constraint in real space, which corresponds to the estimated locations of the signal; a Fourier constraint in reciprocal space, which is the amplitude measured by the detector.

![Figure 1. Principle of the Hybrid Input-Output algorithm.](image)

Coherence of the beam and quality of the detection (signal to noise ratio, dynamic, encoding bits) appear as crucial parameters in the quality of the reconstruction. Nevertheless, experimental design considerations and a good estimation of the support constraint have also their importance.

To yield a unique real space solution, the observed diffraction pattern has to be oversampled at least twice the Nyquist frequency [2, 3], which means practically that the object has to be located and reconstructed in an area at least twice smaller than the real space image frame. This constraint, due to Shannon theorem, is also known as the oversampling ratio, and is fixed by the experimental design according to equation (1). The ultimate resolution of the reconstruction is given by equation (2).

\[
O = \frac{\lambda \cdot d}{a \cdot dx} \geq 2 \quad (1) \hspace{2cm} R = \frac{\lambda \cdot d}{N_u \cdot dx} \quad (2)
\]

where \(d\) is the sample to detector distance, \(\lambda\) the working wavelength, \(a\) the size of the sample under test, \(dx\) the pixel size of the camera and \(N_u\) the size in pixels of the CCD square area containing the diffraction pattern useful information. One may consider a reciprocal space frame size greater than \(N_u\) (\(N > N_u\)), in order to oversample the reconstructed object below the ultimate resolution. But no gain in resolution is to expect by doing so.

The support constraint is calculated from the object autocorrelation function (given by the inverse Fourier transform of the measured diffraction pattern) and the oversampling ratio. In our case, the support constraint is fixed beforehand. However, several kinds of HIO algorithms coexist, most of them refining the support constraint in the course of the convergence [10, 11].

3. CDI experiments
To provide a good understanding of the influence of transverse coherence in CDI reconstructions, we used a well-known amplitude sample under fully and partially coherent illuminations. The sample was a 35 µm thick Gold grid, composed of 3×3 square holes of 8 µm size, over a useful area of 50×50 µm². The holes were rotated by 25° and regularly spaced by 20 µm center to center.

3.1. Fully coherent illumination
For fully coherent illumination of the sample, we used a single-mode fiber laser diode source, emitting light at 400 nm wavelength. The detector was a highly sensitive cooled 14 bits visible CCD camera
(PCO 2000s), with 2048×2048 pixels (7.4 µm/pixel). In order to avoid undesired parasitic reflections and wavefront aberrations inherent to the use of lenses, the setup was realized in the simplest way by sending the source diffraction limited spherical wave directly through the sample onto the CCD camera (Figure 2). Distances were optimized in order to achieve an oversampling ratio of 6.5 and an expected resolution for the sample reconstruction of about 1.1 µm (see equations (1) and (2)).

To increase the signal to noise ratio, we averaged 75 images, with 2 s exposure time each. The resulting image was corrected from background illumination and from residual noise before being processed for CDI reconstruction. Figure 3 shows the experimental results (upper row), and the corresponding theoretical simulations (lower row) obtained in the same geometrical configuration.

One can observe the very good agreement between the measured and simulated diffraction patterns (Figures 3 (a) and (e)), as well as between the autocorrelation functions used for determination of the support constraints (Figures 3 (b) and (f)). The corresponding cross-sections reveal a loss of intensity between the central and edge picks of about 13 % on the experimental measurement (Figure 3 (c)), to be compared to 11 % on the theoretical simulations (Figure 3 (g)). This loss of intensity is only due to the nature of the sample and is not linked to any lack of transverse coherence. Finally, the sample could be reconstructed from the measurement (Figure 3 (d)), with homogeneous illumination of the 3×3 hole array and with an estimated resolution of about 1 µm in accordance with the one expected.

3.2. Partially coherent illumination

For partially coherent illumination, we used the bending magnet source of the Metrology and Tests beamline at SOLEIL. Figure 4 shows the CDI experimental setup as implemented. Spectral selection was performed by the beamline Double Crystal Monochromator (DCM), using two Si(111) Bragg reflections. The monochromatic beam photon energy was fixed at 3 keV (λ ≈ 0.41 nm), and we used a 10 µm thick Iron filter to prevent the sample from parasitic visible light illumination coming from the source. At this energy, spectral resolution is in the range of 10⁻⁴ (i.e. ΔE ≈ 0.3 eV), but higher order harmonic contamination may be important. In order to preserve the temporal coherence required for CDI, we detuned the DCM second crystal from the maximum of the rocking-curve, thus achieving more than 99.8 % spectral purity at the sample position. The divergent beam of the source was sent directly on the sample placed in the beamline endstation; its resulting diffraction pattern was observed downstream by a cooled back-illuminated thinned 16 bits X-Ray CCD camera (Hamamatsu ORCAII-BT-1024G), with 1024×1024 pixels (13 µm/pixel). Distances were optimized in order to achieve an oversampling ratio of 2 and an expected resolution for the sample reconstruction of about 0.32 µm.

Due to the high level of shot noise in this energy range and to achieve a signal to noise ratio better than 100, we averaged 500 CCD raw images, with 500 ms exposure time each. The resulting image was treated for background and noise corrections, before being used for CDI reconstruction of the sample. Experimental results are shown in figures 5 (a), (b), (c) and (d).
Under partially coherent illumination from the synchrotron radiation source, the measured autocorrelation function shows 35% loss of intensity between the central and edge pixels (Figure 5 (c)), while only 11% would have been expected by considering a transverse coherence length greater than the sample size. Moreover, the reconstruction of the sample appears limited to the central hole, with only slight illumination of the nearest neighbors (Figure 5 (d)). In a first approximation, partial coherence effects can be simulated by applying a Gaussian filter to the ideal diffraction pattern. By adjusting the Gaussian convolution kernel to 4×4 pixels, we obtained a similar loss of intensity (about 32%) at the edges of the simulated autocorrelation function (Figure 5 (g)), and a similar partial reconstruction of the sample (Figure 5 (h)). The Gaussian filter applied appears in accordance with the 20 μm transverse coherence length expected at the sample position. One can also observe the very good agreement between experimental and theoretical results. These ones demonstrate the limitations that may occur in CDI reconstruction due to partial coherence illumination.

4. Conclusion

We could perform CDI of a well-known Gold grid at 400 and 0.41 nm wavelengths, demonstrating the efficiency of our HIO algorithm for amplitude objects. Transverse coherence effects on the reconstruction process were studied and compared to theoretical simulations for both fully and partially coherent illuminations. The autocorrelation function calculated from the measured diffraction pattern appears as a useful tool to estimate the degree of transverse coherence at the sample position. Assuming the use of such a reference object, its autocorrelation may be used to perform CDI reconstruction even from partially coherent images.

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