Coherent laser scanning diffraction microscopy

Martin Dierolf¹,², Pierre Thibault¹, Cameron M Kewish¹, Andreas Menzel¹, Oliver Bunk¹ and Franz Pfeiffer¹,²

¹ Paul Scherrer Institut, 5232 Villigen PSI, Switzerland
² École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland
E-mail: martin.dierolf@psi.ch

Abstract. Coherent diffractive imaging (CDI) is a promising approach to high-resolution x-ray microscopy. While CDI typically has a rather limited field of view, this problem can be solved by ptychography, a technique for which an extended object is raster scanned by a compact coherent illumination probe. Significant overlap of illumination for adjacent scan points allows then a self-consistent reconstruction from the entirety of collected coherent diffraction patterns. However, current reconstruction schemes require accurate a priori knowledge of the probe. Our recently developed new algorithm for ptychographic data sets allows us to simultaneously reconstruct both object and illuminating probe. We demonstrate the application of the new method in a test experiment with visible laser light showing that intricate illumination functions can be retrieved reliably.

1. Introduction
In coherent diffractive imaging (CDI) the specimen’s complex-valued transmission function is reconstructed from far-field diffraction intensities by means of phase retrieval algorithms. The achievable resolution only depends on the angular range over which one can detect the diffraction signal. Reconstruction is usually based on an iterative projection algorithm, for instance, the widely used hybrid input-output (HIO) algorithm by Fienup [1] and its variants. To ensure sufficient sampling of the diffraction pattern, either the sample has to be isolated or the illuminating beam has to be confined to a limited region. Although frequently found to be experimentally challenging, the latter approach allows one to obtain images of extended, non-compact specimens by raster scanning. One possibility is to individually reconstruct the diffraction patterns and combine the resulting images afterwards [2]. In contrast ptychography allows a self-consistent, simultaneous reconstruction of the full scanned area from multiple diffraction patterns, given sufficient overlap of adjacent illuminations. Originally developed in the 1970s for electron crystallography [3], ptychography has also been successfully applied to non-crystalline specimens [4–6], recently benefiting from the combination with iterative phase retrieval in the so-called “ptychographical iterative engine” (PIE) [5–7]. However, accurate knowledge of the illumination probe is required a priori or has to be obtained experimentally.

We recently developed a new reconstruction scheme which allows simultaneous reconstruction of both object and illuminating probe [8] from a ptychographic data set. In this article this is demonstrated with visible laser light data collected in a focused-beam geometry.
2. Reconstruction algorithm

The phase retrieval problem for ptychographic data sets can be reformulated as finding the intersection of two sets of constraints. The “Fourier constraint” enforces the Fourier modulus of the object’s exit wave to be consistent with the measured intensities in the diffraction pattern,

\[ I(q) = |\mathcal{F}\{\psi_j(r)\}|^2. \]

The “overlap constraint” states that at each point of the scan the exit wave can be factorized as a illuminating probe \( P \) and a complex-valued object transmission function \( O \),

\[ \psi_j(r) = P(r - r_j)O(r). \]

Exit waves from adjacent scan positions are coupled for non-zero overlap of the corresponding illuminations, which leads to a high redundancy and gives the method its efficiency. The solution of the ptychographic phase retrieval problem, i.e. the two functions \( O \) and \( P \) for which both constraints are fulfilled at each point \( j \) of the ptychography scan, is determined iteratively with the difference map algorithm [9], which uses a combination of projections of the state vector \( \Psi(q) = (\psi_1(r), \psi_2(r), \psi_3(r), \ldots, \psi_N(r)) \) onto the two constraint sets. For the overlap projection

\[ \|\Psi - \Psi^0\|^2 = \sum_j \sum_r |\psi_j(r) - \hat{P}(r - r_j)\hat{O}(r)|^2 \]

has to be minimized, leading to coupled equations for probe and object:

\[ \hat{O}(r) = \frac{\sum_j \hat{P}^*(r - r_j)\psi_j(r)}{\sum_j |\hat{P}(r - r_j)|^2}, \]

\[ \hat{P}(r) = \frac{\sum_j \hat{O}^*(r + r_j)\psi_j(r + r_j)}{\sum_j |\hat{O}(r + r_j)|^2}. \]

For the reconstruction of experimental data, one usually starts with a rough model for the probe \( P \) and a random guess of the object function \( O \). While the updated object function is calculated from equation (3), probe retrieval is achieved by iterating the probe in a nested loop according to equation (4). Updating the state vector \( \Psi(q) \) using the difference map formalism completes one iteration.

3. Experimental

The experimental setup is illustrated in Figure 1: The sample, a cross-section of a pumpkin stem (see Figure 2 for visible-light micrographs), was placed on a scanning stage close to the focal plane of a lens illuminated by a HeNe laser beam (632.8 nm wavelength). A cooled charge-coupled device (CCD) with 1024 × 1024 pixels of 24 × 24 µm² size was placed in the focal plane of a second lens (not shown in Figure 1) to collect far-field diffraction patterns. To compensate for the limited dynamic range of the CCD, five frames with different exposure times were combined for each point of the raster grid. The total scan consisted of 11 × 11 points with 50 µm steps.

The reconstructed images are shown in Figure 3, both (a) the complex transmission function of the object and (b) the probe in the specimen plane. Taking advantage of the chaotic behavior of the difference map algorithm, the images were obtained as averages of 20 reconstruction estimates taken at intervals of five iterations from the steady-state regime of a single run. The pixel size in the reconstruction is 2.6 µm, which is about 45 times smaller than the size of the illuminating probe. The latter corresponds to the intrinsic resolution of this scanning microscope in absence of CDI and shows the potential of the method to overcome instrumental limitations.

The retrieval of the complete illuminating wave field allows us to numerically propagate it to different planes along the optical axis. The longitudinal cut of the propagated probe wave field in Figure 3(c) shows, that the sample was actually placed 1.3 mm upstream from the focus. Although the reconstruction was started with just a disk, resembling a pinhole, this rather complicated illumination function was reliably retrieved.
Figure 1. Experimental setup: The incoming beam is focused onto the specimen forming a small probe. The sample (Figure 2) is scanned perpendicular to the beam. At each point a diffraction pattern is collected with the CCD.

Figure 2. Visible-light micrograph of the specimen, a pumpkin stem cross-section. The magnified square (sidelength 640 µm) corresponds to the field of view in the reconstruction in Figure 3(a).

Figure 3. Reconstruction results, with amplitudes mapped to brightness and phases mapped to hue, see color wheel in (c). (a) Complex optical transmission function of object. (b) Reconstructed probe in the specimen plane. (c) Longitudinal cut of numerically propagated probe wave field.

4. Conclusions
Our new reconstruction approach overcomes the requirement of previous ptychography schemes of accurate knowledge of the illumination, which is hard to model and challenging to characterize experimentally. Complicated illumination functions can be retrieved simultaneously with the object, making the technique perfectly suited for, e.g., combination with scanning x-ray transmission microscopy [8] and use in wavefront-sensing applications.

References
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