

Hard X-ray lensless imaging of extended objects

Lensless X-ray diffraction microscopy is one of the most promising methods for life and material science imaging on the nanometer scale. The high scattering vectors (q -values) available in the Fraunhofer diffraction plane can in principle yield wavelength-limited resolution (i.e. approaching the nm scale), without any of the limitations which apply to X-ray lenses. The key task is to solve numerically for the phase of the scattered intensity.

Solution of the phase problem is rendered tractable via certain iterative phase-retrieval methods. To solve for a given field of view from a single diffraction pattern, the detector must have a pixel size (in the Fraunhofer plane) which is inversely proportional to the size of the object. In terms of practical microscopy, this is a severe limitation: microscopists require the ability to scan a large field of view in order to place an object of interest in spatial context, preferably in real time. Current phase retrieval imaging methods suffer from further limitations. Even if the diffraction plane sampling criterion is satisfied, a unique solution often depends upon the object being single-valued (for example, being a pure phase object or a purely absorptive object). In fact, many objects of practical interest produce both phase and modulus changes onto the exit wavefield. Current methods are also computationally intensive, typically requiring thousands of iterations (each involving two Fourier transforms over the entire - even if limited - field of view), meaning that any possibility of real-time imaging is remote.

We demonstrate here an X-ray microscope which overcomes all of these limitations. We demonstrate a proof-of-principle that X-ray imaging can be accomplished without the need for any sophisticated optics. Given the imminent development of much higher brightness coherent sources (x-ray free electron lasers or XFEL's), we believe the method will open up the possibility of real-time, wavelength-limited hard (or soft) X-ray imaging of objects of any size.

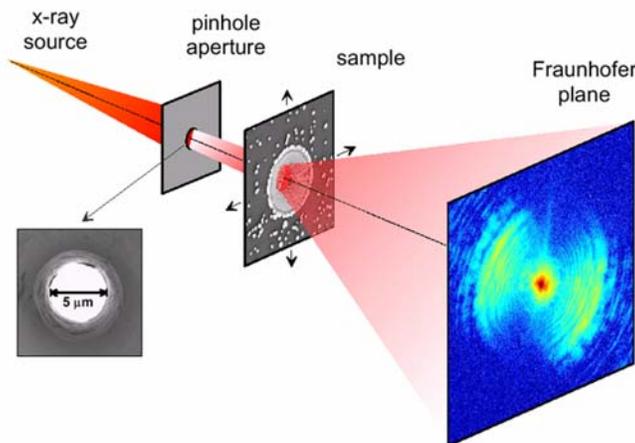


Figure 1: Schematic of the experimental setup for a shifting specimen coherent x-ray diffraction microscopy.

Our experimental approach relies on collecting a number of Fraunhofer diffraction patterns (Figure 1), each of which comes from a different, but overlapping, region of the specimen which is moved laterally across the illuminating beam. The key development is to meld all of these data into a wide field of view. The method is related to a direct (non-iterative) solution of the crystallographic phase problem first proposed by Hoppe. An aperture the size of the unit cell is placed in real space over a periodic object. In the Fraunhofer diffraction plane, each crystalline reflection is now convoluted with the Fourier transform of the aperture function. In one dimension, such an aperture is a 'top hat', hence

the diffracted peaks are convoluted with *sinc* functions. At their point of overlap, the *sinc* functions add according to the complex values determined by the phase of the underlying diffracted beams. The intensity of each adjacent diffracted peak is easily measured: the intensity at the mid point (the ‘in-between diffraction spots’, nowadays referred to as the ‘over-sampled’ diffraction spots) gives a measure of their relative phase. Hoppe recognized that this measure could still lead to an ambiguity of a complex conjugate in each diffracted beam, as is usual in the classic phase problem. However, by moving the aperture function to a new position displaced by less than one unit cell, a new measure can be obtained for this phase difference, and hence all phases are obtained un-ambiguously. This method, relying on a convolution (or ‘folding’) in reciprocal space was later called ‘ptychography’ (from the Greek ‘ $\pi\tau\upsilon\xi$ ’, meaning to fold). While it may not be obvious, ptychography is helpful for extended non-crystalline objects and in fact many of its benefits still apply. Our iterative technique incorporates this ptychographic phase data to piece together a large field of view (see [1] for more details).

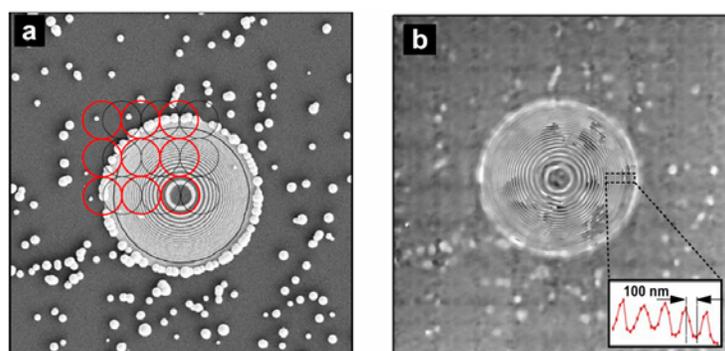


Figure 2: Experimental results for a test object with gold balls. (a) A scanning electron micrograph of the test sample containing gold balls and a lithographically produced zone plate. The circles indicate 18 of the 289 probe positions for which diffraction patterns were recorded. (b) Reconstructed phase image displayed on a linear grayscale ranging from $-\pi$ to $+\pi$. The insert in (b) is a profile through the outermost rings of the zone plate which have a width of 100 nm).

As an example, the reconstructed phase of a test object - a Fresnel zone plate with gold balls - after 50 iterations is shown in Figure 2. On the outskirts of the zone plate, the alternating attenuating and phase shifting concentric rings in the center of the image, is a random distribution of gold balls ranging from 250 to 1500 nm in diameter. Both the ring structure and the outlying gold balls are clearly visible in both the reconstructed modulus and phase.

We believe that this method can be readily and routinely be applied to life science microscopy, e.g., for imaging cells or cellular substructures at 10 nm resolution or better. The technique can in principle deliver wavelength-limited resolution without the use of any high-precision optical elements, although to achieve this ultimate goal will require a very high brightness source (so that appreciable intensity will be scattered at large angles), of the sort expected to become available at x-ray free electron lasers.

Publications

- **Hard X-ray lensless imaging of extended objects,**
J. M. Rodenburg, A. C. Hurst, A. G. Cullis, B.R. Dobson, F. Pfeiffer, O. Bunk, C. David, K. Jefimovs, and I. Johnson*
[PHYS. REV. LETT. **98**, 034801 \(2007\)](https://doi.org/10.1103/PhysRevLett.98.034801)
<http://dx.doi.org/10.1103/PhysRevLett.98.034801>

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