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Soft X-ray Diffraction Tomography: Simulations and First Experimental Results

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Abstract. Diffraction tomography allows us to obtain high-resolution 3D phase and amplitude reconstructions of thick specimens. Here we report on some difficuties arising in the experimental realization of diffraction tomography. These initial experiments together with computer simulations are presented and first results obtained by incorporating the suggested modifications are shown for a collection of 1 μm diameter latex spheres and a 3 μm diameter gold dot.

1. INTRODUCTION

Conventional tomography is based on the collection of simple projection images of a specimen over a range of rotation angles, with an invertible relationship between image contrast and projected object thickness. This approach can even work in a microscope, provided that the specimen is within the depth of focus, and has delivered 100-200 nm 3D images of biological specimens [1-3]. However, the transverse resolution for a microscope is $\delta_t=0.61\lambda/(N.A.)=1.22\delta_{rN}$, while the depth of focus is $DOF=2\lambda/(N.A.)^2=8(\delta_{rN})^2/\lambda$, where δ_{rN} is the outermost zone width of the zone plate. A typical depth of focus would be only 2 μm if δ_{rN}=20 nm zone plates were to be used at the 2.3 nm wavelength; this thickness would be completely inadequate for most biological cells. With such a short depth of focus, the sample thickness gain of x-ray microscopy over electron microscopy would be minimal.

One solution to this dilemma is not to record images, but to record holograms of the specimen [4]. While the focused image obtained from a hologram has no better depth resolution than a conventional image obtained using the same numerical aperture, the hologram can be focused to examine many depth planes while the conventional image cannot. Because the depth resolution is unchanged, tomography must still be used: it is necessary to record holograms under different tilt angles to reconstruct the 3D structure of the specimen. This approach is known as diffraction tomography. It is important to note that these multiple holograms solve a longstanding problem with in-line or Gabor holography; namely, they eliminate the twin image. In a nutshell, the backpropagation of the complex amplitudes involves *real* holographic images that reinforce each other since they all represent measurements of the specimen. However, the *virtual*, or twin, images tend to cancel each other out. This effect is enhanced if one can record holograms at two different recording distances for each tilt angle. This method has been nicely demonstrated in optical experiments by A. Devaney and collaborators [5, 6] and more recently with hard x-rays at micrometer resolution by P. Cloetens and collaborators [7].

Since a hologram also contains information about the phase contrast of a specimen (which is dominant, especially at X-ray energies above 1 keV), diffraction tomography offers important added information about the 3D amplitude *and* phase of the object. The reconstruction process involves back*propagation* of a complex wavefield from each hologram. Experimentally, diffraction tomography can be done by magnifying the far-field hologram with a zone-plate onto a CCD camera (Figure 1), which allows fast data acquisition. It is also necessary to record holograms under different tilt angles to reconstruct the 3D structure of the specimen.

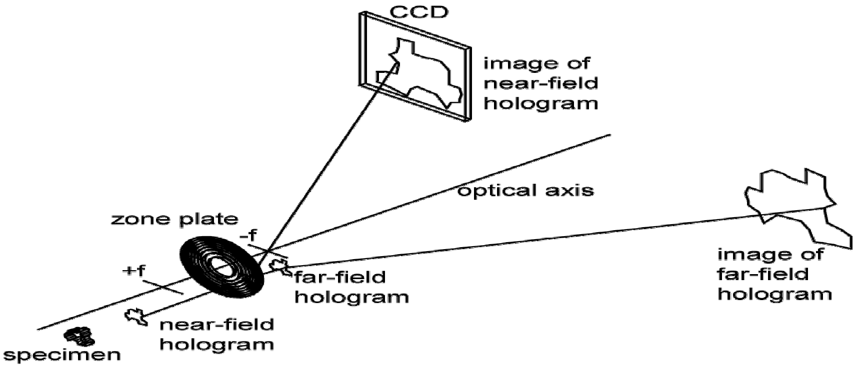


Figure 1: Schematic of a geometry for recording two in-line holograms for diffraction tomography using a zone plate for magnification onto a CCD detector.

2. INITIAL EXPERIMENTS - EFFECTS FROM THE ZONE PLATE AND COMPUTER SIMULATIONS

The inital experiments made use of a zone plate without a central stop so that the object could be placed close to the optical axis. Such an arrangement made it possible to simultaneously record the image of the far-field and near-field hologram on the CCD. Figure 2 shows obtained holograms of 1 μm diameter latex spheres. The upper part of the CCD image shows the almost in-focus image formed by the positive first order focus. The lower part shows the far-field hologram formed by the negative first order focus. The intense straight x-ray beam is partially blocked out by a wire beamstop. The recorded image clearly shows strong fringes around the zero order beam. These fringes make it difficult to collect high quality data and further complicate the reconstruction. We note here that the sample was prepared at the edge of a SiN_3 window so that a clear separation of the positive and negative order image was achieved.

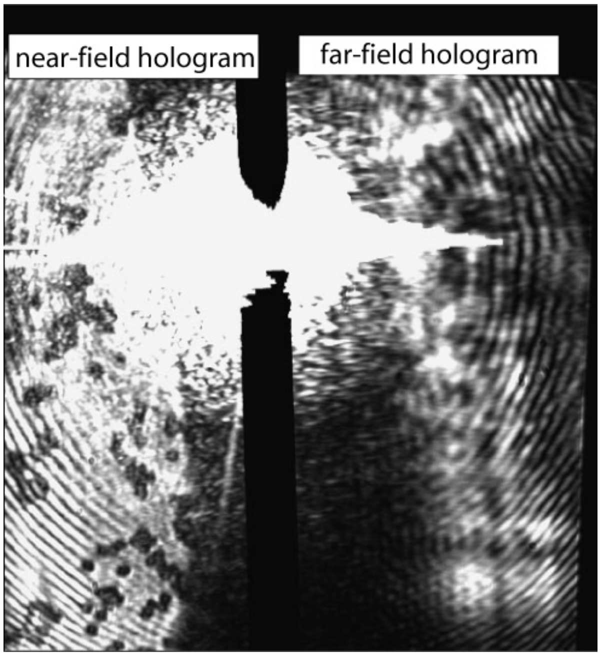


Figure 2: Experimental schematics of diffraction tomography. A Fresnel zone-plate magnifies wavefields from different propagation distances onto the detector plane.

In a second experiment the latex spheres were replaced by a pinhole and the CCD camera was positioned slightly off-axis. Such an arrangement made it possible to allow for larger offsets between the pinhole and the zone plate. Figure 3 a) shows a recorded image of the pinhole using the first-order focus of the zone plate. Fringes across the image of the pinhole are visible again. As the zone plate is moved farther off-axis the image becomes much cleaner (Figure 3 b)). The image formed by the negative first-order focus was obtained by moving the zone plate opposite of the optical axis and is shown in Figure 3 c).

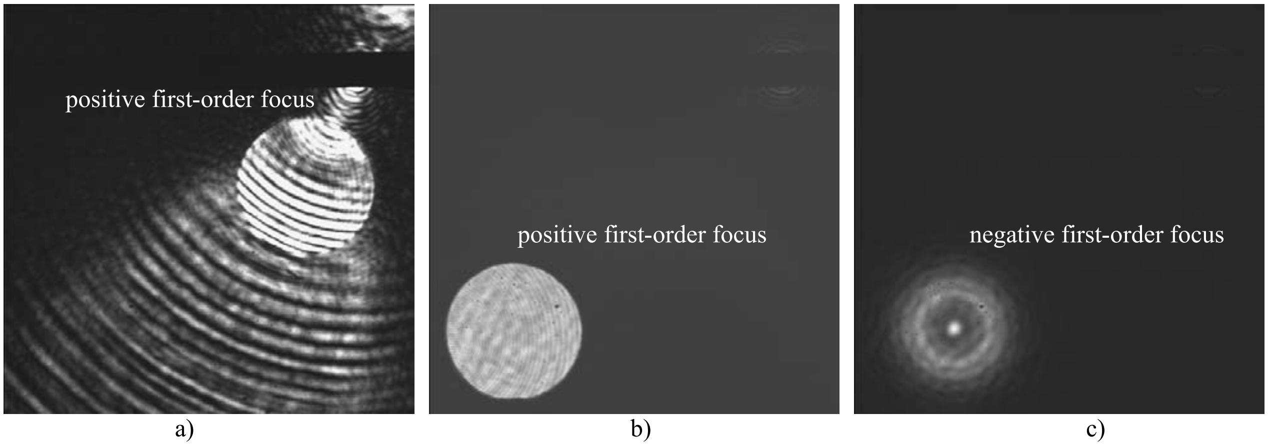


Figure 3: Experimental data: images of a pinhole for two different zone plate offset distances (a,b) using the positive first-order focus. c) image of pinhole using the negative first-order focus.

In order to understand the cause of the fringes, we simulated the experiment on a computer using the IDL language. Assuming plane wave illumination (constant phase across the pinhole) the program simulates a pinhole and propagates the wavefield to the plane of the zone plate. A zone plate with absorption and phase shift is generated and shifted by a certain distance to simulate the off-axis configuration. Absorption and phase shift due to the zone plate is applied to the wavefield and the Fourier transform is taken to simulate the image at the detector plane following Goodman [8].

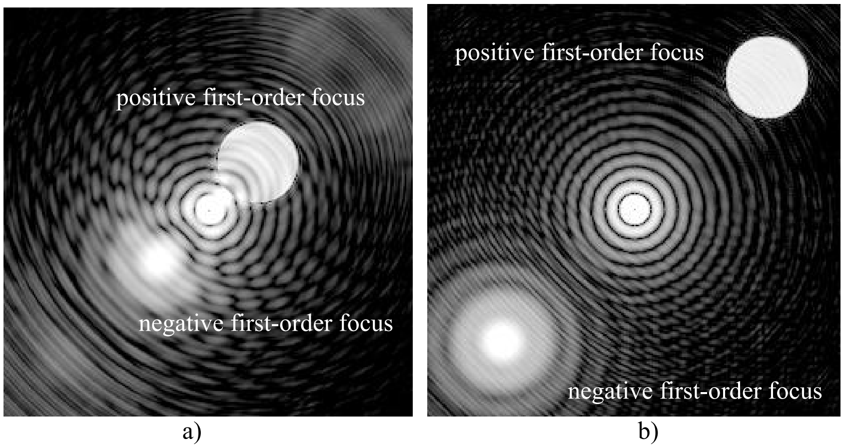
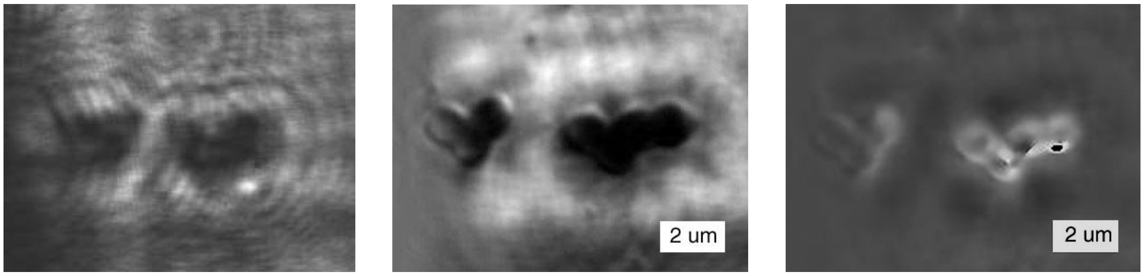


Figure 4: Simulated data: images for two different zone plate offset distances.

The simulated data images are shown in Figure 4 for two different zone plate offsets. The images are in agreement with the experimental data and show that the fringes become less visible as the zone plate is moved farther off-axis. We believe that the fringes are caused by the fact that the coarseness of the innermost zones provides a poor local approximation to the desired continuous phase function of a lens. We have therefore attempted to move the zone plate farther away from the optical axis so as to use in the beam path the much greater number of finer zones at larger zone plate radii. Figure 4 c) shows the same simulated imaging geometry but with a lens instead of a zone plate to form the magnified image of the object.

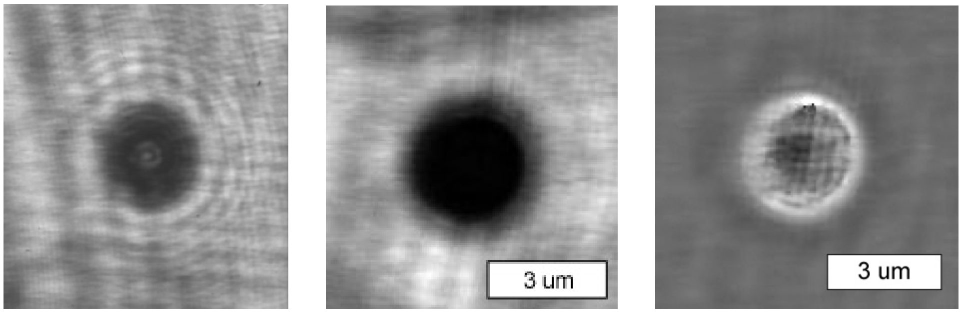
3. FIRST EXPERIMENTAL RESULTS

The first experiments at 390 eV were carried out using the Stony Brook STXM with a modification to accommodate a liquid nitrogen cooled CCD camera. Holograms of 1 μm diameter latex spheres (Figure 5 a)) and a 3 μm diameter gold dot (Figure 6 a)) were recorded at several propagation distances. The holograms were reconstructed by backpropagation and the complex wavefields of the reconstructions were summed to yield a 2D reconstruction of the object. Figure 5 shows the reconstructed intensity (b) and phase (c) for the latex spheres. Figure 6 shows the reconstructed intensity (b) and phase (c) for the gold dot.



a) b) c)

Figure 5: Hologram a) and reconstruction of intensity b) and phase c) of the 1 μm diameter latex spheres.



a) b) c)

Figure 6: Hologram a) and reconstruction of intensity b) and phase c) of the 3 μm diameter gold dot.

We note here that the quality of the data and therefore also the quality of the reconstruction is not outstanding. This was due to experimental geometry constraints that arose due to fitting this experiment into the Stony Brook STXM apparatus. These constraints will be removed in a new apparatus that is now being commissioned, which is described in an accompanying paper in these proceedings [9]. This apparatus includes a CCD camera with more pixels and a cryo transfer system for work with biological specimens, and it is being designed to allow for automated data collection of holograms over a rotation series to carry out experiments in diffraction tomography.

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