Phase retrieval in x-ray lensless holography by reference beam tuning

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We show the ability to determine the relative phase between the object and a reference scatterer by tuning the overall intensity and phase of the reference wave. The proposed reference-guided phase retrieval algorithm uses the relative phase as a constraint to iteratively reconstruct the object and the reference simultaneously, and thus does not require precisely defined reference structures. The algorithm also features rapid and reliable convergence and overcomes the uniqueness problem. The method is demonstrated by a soft-x-ray coherent imaging experiment that utilizes a large micrometer-sized reference structure that can be turned on and off, yielding an object image with resolution close to the reconstruction pixel size of 21 nm. © 2009 Optical Society of America

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At the heart of holography lies the relative phase, which is encoded in the interference fringes produced by coherent superposition of the reference and the object waves. The object phase can be recovered to the extent of the knowledge of the reference phase, but in the x-ray regime this has been impeded by the lack of suitable optics to create and control reference beams. Consequently, most efforts in x-ray holography have pursued lensless approaches. In the past decade, a few studies have demonstrated the power of utilizing nanoscale reference structures [1–3]. However, in these approaches the image resolution and the quality of the image reconstruction depend on the ability to create well-defined, ultrasmall reference structures, typically produced by nanofabrication.

In this Letter we introduce an alternative by incorporating traditional phase retrieval [4,5] into x-ray holography. Instead of relying on the precise fabrication and knowledge of the reference structure, we use an extended reference whose transmissivity can be tuned, e.g., by changing the incident wavelength. Recording multiple holograms with varying overall reference intensity and phase allows us to determine the relative holographic phase. This phase information serves as a Fourier domain constraint in an iterative algorithm to recover the image. The proposed reference-guided phase retrieval (RPR) method deconvolves the object and the reference simultaneously. The holographic constraints ensure that the convergence is rapid and independent of the signal-to-noise ratio (SNR). This is in contrast to previous work [3,6–8], where improvements in the resolution beyond the reference size are achievable by subsequent application of phase retrieval algorithms only when the SNR is sufficient. Our technique builds on earlier work that demonstrated multiple-wavelength anomalous diffraction near absorption edges for the reconstruction of nonperiodic objects [9]. Here, we generalize this concept and show that it is suitable for recovering phases in a broad range of lensless imaging scenarios.

Consider the exit wave at the sample plane taking the form \( \psi(x, y) = \psi_o(x, y) + \xi \psi_r(x, y) \), where \( \psi_o \) and \( \psi_r \) describe the scattered waves from the object and the reference, respectively, and the complex-valued parameter \( \xi = |\xi|e^{i\phi} \) represents a tunable reference. In the Fraunhofer diffraction regime the wave field can be written as

\[
\Psi(p, q) = \Psi_o(p, q) + \xi \Psi_r(p, q),
\]

(1)

where \( \Psi(p, q) \) denotes the Fourier transform of \( \psi(x, y) \), and \( (p, q) \) are the reciprocal space coordinates. The diffraction intensity is given by

\[
I(p, q) = |\Psi_o|^2 + |\xi|^2|\Psi_r|^2 + 2|\Psi_o||\Psi_r||\xi|\cos(\Delta\Phi + \phi),
\]

(2)

where \( \Delta\Phi(p, q) = \Phi_o(p, q) - \Phi_r(p, q) \) is the relative phase of the object and the reference wave in reciprocal space. By tuning \( \xi = \xi_1, \xi_2, \xi_3, \ldots \) and recording three or more diffraction patterns as a first step, the three unknowns \( |\Psi_o|, |\Psi_r|, \) and \( \Delta\Phi \) can be determined for each point \( (p, q) \). These components form the Fourier domain constraints for the RPR routine, as shown in Fig. 1.

As a second step, the RPR routine iteratively deconvolves the object and the reference by determining their individual phases \( \Phi_o \) and \( \Phi_r \). As shown in Fig. 1, the algorithm starts with a random guess for \( \Phi_o \) and uses the error reduction method [4] on the object to update the object’s phase to \( \Phi'_o(i) \). Because of the Fourier domain constraints, the phase of the reference is updated as well, i.e., \( \Phi'_r(i) = \Phi'_o(i) - \Delta\Phi \). Applying another error reduction cycle, this time on the reference, gives \( \Phi'_r(i+1) \) and \( \Phi'_r(i+1) = \Delta\Phi + \Phi'_r(i+1) \). The RPR routine iterates until the update falls below
a given threshold. The embedded error reduction uses the amplitudes \(|\Psi_r\rangle\) and \(|\Psi_o\rangle\) and support regions defined by the autocorrelations as the Fourier and the object domain constraints.

To investigate the convergence characteristics of the algorithm, we choose a real-valued test structure, shown in Fig. 2(a), with a large circular reference placed next to it. Assuming knowledge of \(|\Psi_o\rangle\), \(|\Psi_r\rangle\), and \(\Delta \Phi\), the convergence is quantified by calculating the normalized mean square error (NMSE) after each iteration \(i\),

\[
\text{NMSE}_i = \frac{\sum |\psi_i - \psi_o|^2}{\sum |\psi_o|^2},
\]

where \(\psi_o\) is the convergence limit for the object. The image quality associated with typical NMSE values are shown in Fig. 2(b). The convergence of RPR and the hybrid input-output algorithm (HIO, a standard phase retrieval algorithm for single diffraction patterns \([5]\), using \(|\Psi_o\rangle\), \(|\Psi_r\rangle\), and \(\Delta \Phi\), are spatially separated in the Fourier transform of \(I_o\) to compensate for the change in wavelength, we derive \(|\Phi_o\rangle\), \(|\Phi_r\rangle\), and \(\Delta \Phi\) from two instead of three holograms: \(I_o = |\Psi_o|^2\) and \(I_r = |\Psi_r + \Psi_o|^2\), where the autocorrelation and the cross-correlation terms, corresponding to \(|\Psi_o|^2\) and \(2|\Psi_r||\Psi_o|\cos \Delta \Phi\), are spatially separated in the Fourier transform of \(I_o - I_r\).

We performed the experiment at the Stanford Synchrotron Radiation Lightsource (SSRL), beamline 13-3. The two diffraction patterns are recorded at 775 eV(\(I_{\text{eV}}\)) and 765 eV(\(I_{\text{eV}}\)), as shown in Figs. 3(c) and 3(d) with a \(1340 \times 1300\) pixel CCD detector placed 250 mm from the sample. Two beam stops of

As a proof-of-principle experiment, we applied the RPR scheme for nanoscale imaging with Fourier transform holography (FTH) \([1,2]\), using a micrometer-sized reference aperture that can be switched on and off. The object and the reference aperture are placed in the FTH geometry as shown in Fig. 3(a). The test object and a reference are fabricated by focused ion milling. The diameter of the 1 µm circular aperture is chosen for optimum fringe visibility in the hologram. A 200 nm Co film [see Fig. 3(b)] serves as a shutter to switch the reference scattering on (\(\varepsilon = 1\)) and off (\(\varepsilon = 0\)) by changing resonantly the absorption around the Co L\(_3\) edge. After resizing \(I_{\text{eV}}\) to compensate for the change in wavelength, we derive \(|\Phi_o\rangle\), \(|\Phi_r\rangle\), and \(\Delta \Phi\) from two instead of three holograms: \(I_{\text{eV}} = |\Psi_o|^2\) and \(I_{\text{eV}} = |\Psi_r + \Psi_o|^2\), where the autocorrelation and the cross-correlation terms, corresponding to \(|\Psi_o|^2\) and \(2|\Psi_r||\Psi_o|\cos \Delta \Phi\), are spatially separated in the Fourier transform of \(I_{\text{eV}} - I_{\text{eV}}\).

We further introduce shot noise to the simulated holograms for investigating the influence of photon counting noise on RPR. Without loss of generality, we set \(\xi = 0, 1, 2\) in Eq. (2) to obtain \(|\Psi_o\rangle = \sqrt{I_o}\) \(|\Psi_r\rangle = \sqrt{I_r}\) \(|\Psi_o\rangle = \sqrt{(I_o - 2I_1 + I_2)}/2\) and the relative phase

\[
\Delta \Phi = \arccos\left(\frac{-3I_0 + 4I_1 - I_2}{2\sqrt{2I_0(I_o - 2I_1 + I_2) + \sigma}}\right),
\]

where \(\sigma\) is the Wiener filter parameter to reduce the effect of zero crossings \([10]\). A correction method is then applied to unwrap the phases \([11]\). As shown in Fig. 2(d), for total photon counts ranging from \(10^6\) to \(10^{10}\), noise lowers the final image quality as reflected in the final NMSE values reached. However, convergence speed is independent of the noise level. In addition, minor deviations in \(\xi\) do not affect the outcome of RPR.

![Image](image_url)
RPR reduces the requirements for both accurate knowledge and precise fabrication of the reference structure. Here, the dimensions of the reference can be selected for optimum fringe visibility in the hologram. Various experimental schemes to obtain multiple holograms for RPR are conceivable. Illumination control can be integrated by other means such as microelectromechanical systems. The tuning of interference can also be achieved by changing object scattering such as in multiple-wavelength anomalous diffraction holography [9], which uses the in-line holography geometry.

In conclusion, we have proposed a phase retrieval algorithm for lensless x-ray microscopy, where the phase difference derived from multiple holograms is introduced as an additional constraint in the Fourier domain. This implementation is reliable and robust against noise and dramatically increases the reconstruction convergence speed. The potential and feasibility of RPR is experimentally verified.

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References