A direct approach to coherent diffractive imaging

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Coherent diffractive imaging is an imaging technique that seeks to restore the exit-surface wave of the object being imaged from intensity measurements, either in the diffraction plane or the Fresnel diffraction region. To date numerous strategies have been proposed to complete this restoration, the most successful being the original scheme proposed by Gerchberg and Saxton [1] and its subsequent modifications. These schemes all involve the iterative refinement of a trial wave function using a priori known information about the sample to constrain the phase in conjunction with the measured amplitude. These are nonconvex, nonlinear optimisation problems and as such are plagued by uniqueness issues. In parallel to these conventional nonlinear methods there has been significant effort directed toward deterministic methods. Here we consider a generalisation of holography proposed by Martin and Allen [2] which transforms the CDI phase problem into a set of linear equations that has a definite and unique solution.

Consider the diffraction pattern of a gnat’s wing shown in Fig. 1(a), formed using the imaging geometry in Fig. 1(b). It is possible to solve for the exit-surface wave, in the area around the object indicated by the line in Fig. 1(b), from the autocorrelation of the exit-surface wave (obtained from the inverse Fourier transform of the diffraction pattern). To do so we write the exit surface wave as a sum of the illumination and the modification to the illumination arising as a result of it passing through the object. Following the procedure outlined in [2] it is possible to set up a system of linear equations from the autocorrelation of the form $Ax = b$. The matrix $A$ is constructed entirely from the known illumination and $b$ is taken from the regions of the autocorrelation which are linearly related to the unknown object function. A proof of principle of this method at high fidelity was recently published by Morgan et al. [3]. This involved a system of 311632 linear equations for 51026 unknown variables (the amplitudes and phases). The solution of this set of equations using the standard QR or SVD decomposition is both memory and time intensive. We have introduced a fast, dependable algorithm to solve the linear equations which has a small memory requirement and is computationally very fast [4]. The algorithm is based on the conjugate gradient least squares method to give an iterative solution and is known to converge in a predetermined number of steps. Each iterate of the algorithm, dubbed iterative linear retrieval using Fourier transforms (ILRUTF), requires only a handful of fast Fourier transforms. Using this approach the results in Figs. 1(c-f) were obtained.

We have recently applied this approach to achieve an atomic resolution reconstruction of a region of a cerium dioxide film illuminated by a coherent scanning transmission electron microscopy probe. This single-shot approach to retrieving the exit-surface wave should be contrasted with recent atomic-resolution ptychographic reconstructions which rely on multiple overlapping probe positions for their success [5,6]. The key point is that the approach discussed here is very robust with respect to noise since regularization by iteration number is possible - the first iterations retrieve the essential structure before measurement noise in the data can overwhelm the retrieval. These preliminary results are shown in Fig. 2, where the high-angle annular dark-field (HAADF) image of the cerium dioxide nanoparticle is overlaid with two reconstructions done independently from separate rochigrams (diffraction patterns). Shown in each case is the phase of the retrieved exit wave divided by the illumination function. Only the heavier cerium atoms are evident in the reconstructions. However there is evidence for cerium atoms at the edges of the specimen which are not revealed by the HAADF image. The standard nonlinear phase retrieval approaches are not as successful under the same set of assumptions, since they tend to be affected by the noise in the single input rochigram in a way which compromises them from the outset.
References

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Figure 1. Proof of principle. (a) Diffraction pattern of a gnat’s wing and (b) high resolution microscope image showing the circular illumination used in ILRUFT. The retrieved (c) amplitude and (d) phase after a single iteration of ILRUFT and (e) amplitude and (f) phase after 50 ILRUFT iterations.

Figure 2. The HAADF image of a cerium dioxide nanoparticle overlayed with two independent ILRUFT reconstructions from different ronchigrams (diffraction patterns). Shown in each case is the phase of the retrieved exit wave divided by the illumination function.