Boundary-artifact-free phase retrieval from Differential Phase Contrast image

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The differential phase contrast (DPC) imaging in STEM becomes a hot topic, since the possibility of the DPC imaging at atomic resolution has been demonstrated using a segmented detector (a concentric quadrant detector) [1]. The idea of the DPC imaging in STEM was proposed by Dekker and de Lang [2] and mainly used for a study of magnetic material in a medium resolution [3]. Waddell and Chapman [4] demonstrated that the first moment of the diffraction distribution is proportional to a gradient of the object phase for a pure phase object. They showed that the split detector (a set of two semicircular detectors) gives an approximate to the first moment perpendicular to the split line. Using a quadrant detector we can obtain two perpendicular components of the first moment. Recently, fast acquisition of 2D diffraction data becomes possible and we can get a real first moment at each scan position using so-called 4D-STEM technique. Thus, the DPC opens up the possibility to retrieve the object phase, which is proportional to a projected electric potential. We have developed a DigitalMicrograph plug-in, called qDPC (quatitarive DPC), which can handles the signals from a segmented detector as well as a pixel detector.

We may note that we have to retrieve the object phase that satisfies simultaneously two DPC signals. Close et al. proposed the formula for the phase by combining the two DPC signals in Fourier space [5]. Lazic et al. proposed the formula corresponding the Poisson equation for the phase in Fourier space [6]. The solution of these formulas is usually obtained by using fast Fourier transform (FFT). However, the FFT assumes the periodic boundary condition that will often introduce an unwanted background. Although the boundary condition in general cannot be measured, in our case our observables (DPC signals) are the differentials of the solution. Thus, we can use the Neumann boundary condition that is the differentials of the solution perpendicular to the boundary. In this case, the eigenfunction is cosine, and we can use the discrete cosine transform (DCT) instead of the solver based on the FFT. Here, we emulate the DPC signals as the derivatives calculated along x- and y-directions of the model (Fig. 2a), and add the noise whose size is 10% of the full range of each derivative. Figure 1 compares the results obtained with the DCT and two FFTs. The results obtained by FFT show slowly varying artifact added to the model contrary to the result obtained by DCT.

We have also developed the real-time routine that directly integrates the observed two DPC signals. Our real-time routine estimates a reliable value by integrating over many paths and updates the phase map during the progress of the scan. Figure 2 shows the results obtained by a simple integration and the multi-path integration. Here, the size of the noise is also 10% of the range of each derivative.

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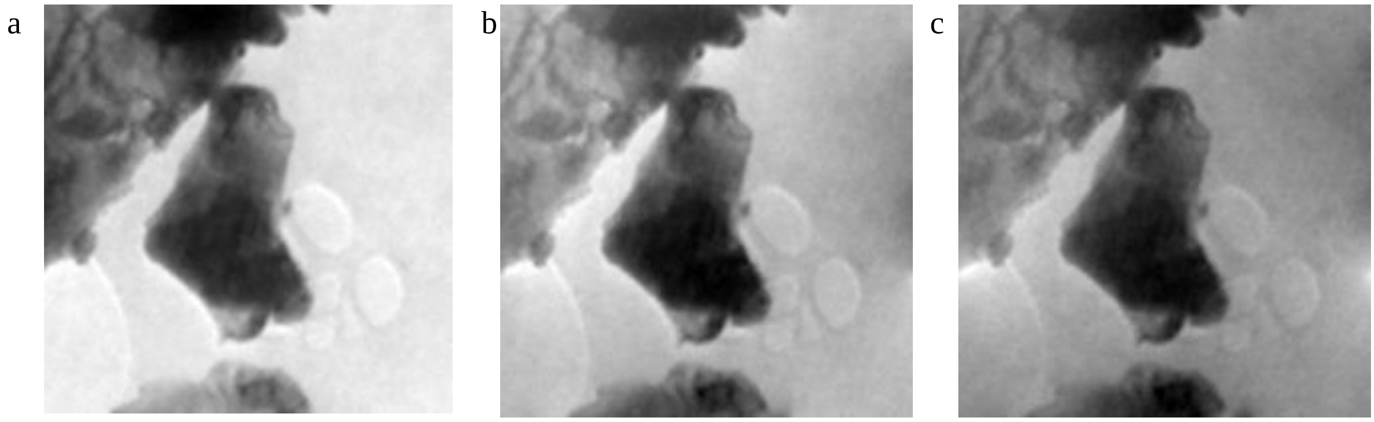

Figure 1. Retrieved maps obtained from the x- and y-derivatives using (a) DCT (this study), (b) FFT [5] and (c) FFT [6]. (see Fig. 2a for the original data)

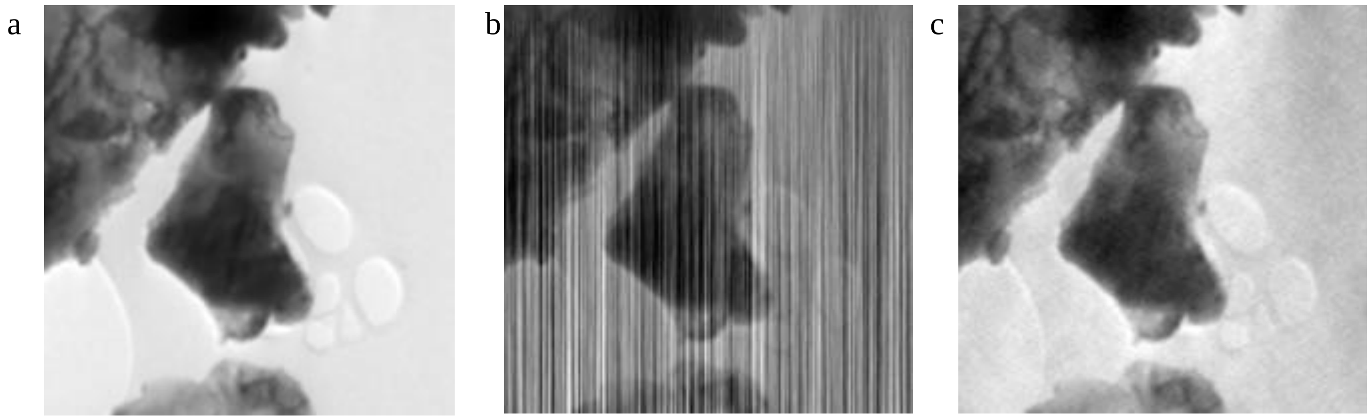

Figure 2. Real-time integration from the x- and y-derivatives. (a) Original model data. Retrieved maps obtained by (b) the simple routine that integrates along the vertical direction and (c) the new routine that integrates on multiple integration paths.