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How many detector pixels do we need for super-resolution ptychography?

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In traditional scanning transmission electron microscopy (STEM) imaging, the spatial resolution limit is set by the diffraction limit from the probe-forming aperture. This limit can be overcome by ptychography, where we collect a 4-dimensional dataset consisting of a diffraction pattern (kx, ky) at each scan position (x, y) for phase reconstruction. With the development of iterative phase retrieval algorithms such as ePIE and high dynamical range pixel-array detectors that enable the acquisition of the full scattering distribution, images with usable information beyond the diffraction limit have been achieved [1]. One challenge for ptychography is the relatively slow acquisition speed of the 4D dataset – 0.1-1 ms/real space position compared to 0.1-10 μs for differential phase contrast (DPC) imaging with a quadrant i.e. (2x2) detector. The longer acquisition times lead to more noticeable scan noise, drift and damage. Here, we demonstrate that super-resolution ptychography is still possible with only 2 × 2 detector pixels when the real space sampling is sufficient and that the ptychography can significantly outperform the conventional DPC analysis. Smaller detectors such as segmented detectors are much faster thus we now open up the possibility of using such faster detectors for ptychography[2].

The ptychographic sampling ratio $S_{x,y} = 1/(UR)$, where U is the reciprocal space sampling and R is the real space sampling, is the criterion that determines the quality of electron ptychography phase reconstruction [3]. For the same quality of reconstruction, we can trade-off the reciprocal space sampling for increased real space sampling. Given fewer detector pixels, to compensate for the diffraction patterns undersampling with respect to Nyquist detector sampling, an oversampling in real space is therefore required. We explored the effect of $S_{x,y}$ on the resolution by varying the probe scan step size and the detector-pixel number in the simulated 4D-STEM datasets. Figure 1 shows that diffraction datasets with more than 8 × 8 detector pixels still give good reconstructions, but when the diffraction dataset has only 4 × 4 detector pixels, the reconstructed image contrast is degraded.

However, as $S_{x,y} = 8$ is still large, a reconstruction should still be possible. In fact, a reciprocal space upsampling in the phase retrieval processing is very useful, because it helps to access the data redundancy from probe positions in the object plane, provided $S_{x,y} >> 1$ [4]. Virtual detector subpixels can be enabled for undersampled diffraction patterns by interpolating the diffraction patterns and normalizing intensity within each original detector pixel after the estimate of the exit wave in each iteration of ePIE [4]. Using subpixel upsampling in ePIE, a good phase reconstruction from 2 × 2 detector pixels is accomplished (Fig. 1f), which otherwise would fail to give meaningful structures.

A resolution comparison between conventional integrated DPC (iDPC) [5] and ptychography, both using the same 2 × 2 detector pixels is displayed in figure 2. For the same 2 × 2 detector dataset, ptychography performs better in resolving the Si dumbbell structure – both in terms of FWHM and dip between adjacent atoms, which means 4 detector-pixels are sufficient to maintain super-resolution ptychography. The

significant reduction of pixel numbers enables the usage of fast segmented detectors for ptychography. [7]

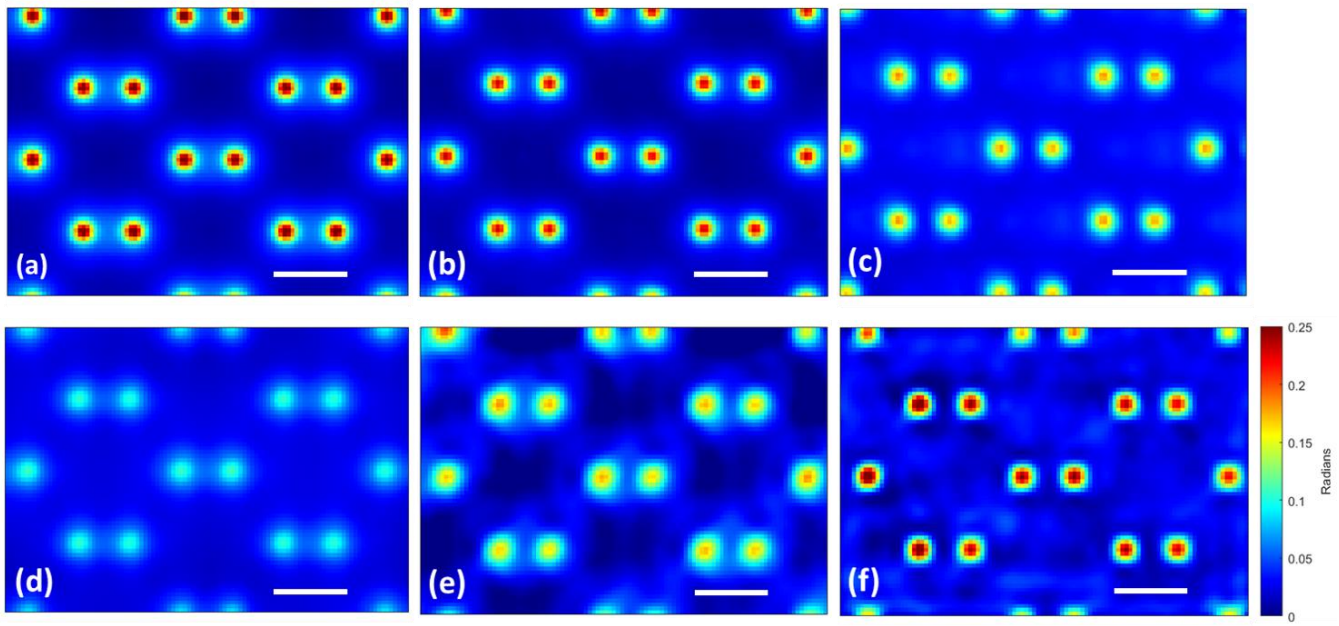

Figure 1. Figure 1. 4D-STEM ptychographical phase retrieval of Si (110) dumbbell structure by ePIE as a function of detector pixels. (a) Reconstruction from 64 × 64 detector-pixels with Sx,y = 132 has excellent resolution. (b) Reconstruction from 16 × 16 detector-pixels with Sx,y = 33 still has good resolution. (c) Image contrast reconstructed from 8 × 8 detector-pixels with Sx,y = 17 has degraded. (d) Image contrast reconstructed from 4 × 4 detector-pixels with Sx,y = 8 has further degraded. (e) With 16 times upsampling to 64 × 64 pixels, image contrast reconstructed from 4 × 4 detector-pixels with Sx,y = 8 has only minor artifacts. (f) With 32 times upsampling to 64 × 64 detector pixels, image contrast reconstructed from only 2 × 2 detector-pixels (Sx,y = 4) is recovered. All simulated 4D-STEM datasets have the same probe scan step size 0.102Å but a different number of detector pixels. The 4D-STEM dataset was simulated at 300kV beam voltage, 24 mrad convergence angle α and Scherzer defocus with 0.01mm spherical aberration, on the single-unit cell thickness Si (110) plane with 2α maximum scattering angle by μSTEM [6]. The scalebar is 2Å and colormap is the same for all the images.

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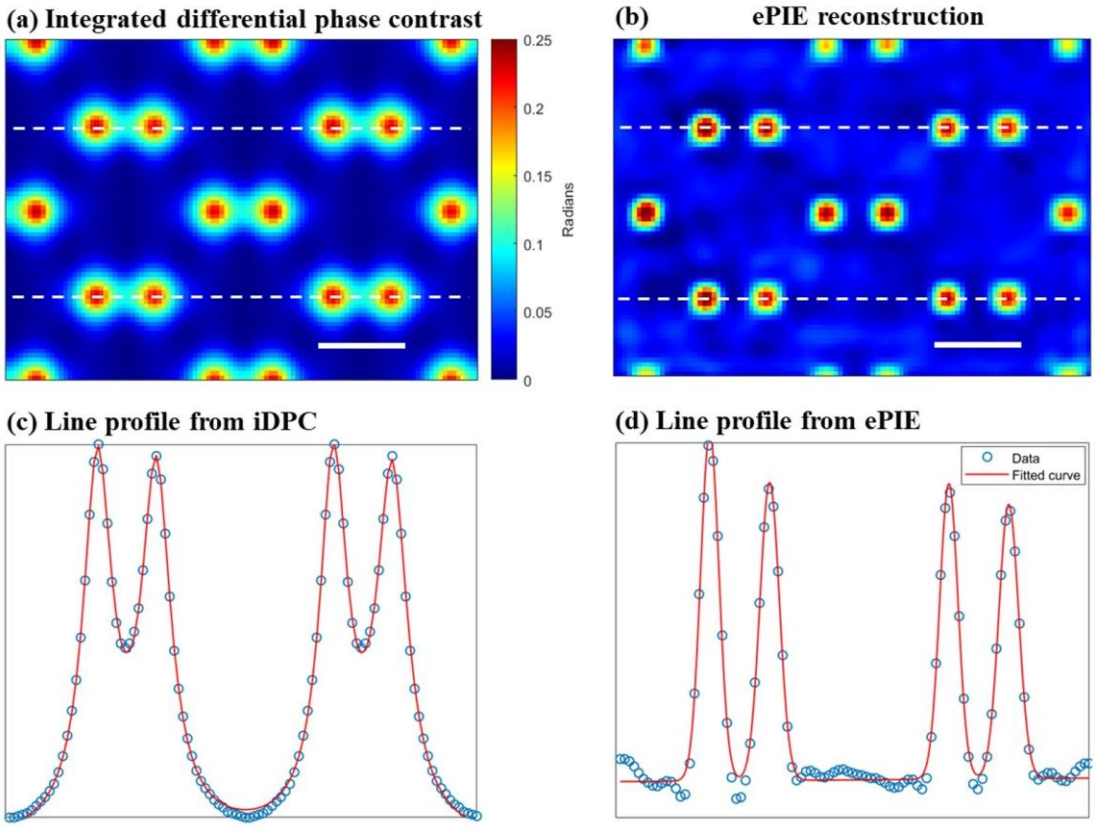

Figure 2. Figure 2: Phase contrast images of Si (110) dumbbell structure reconstructed by integrated differential phase contrast (iDPC) and ptychographical iterative engine (ePIE) using the same 2 × 2 pixels detector 4D-STEM dataset. Fig. 2c& 2d) show line profiles at the position of white dashed lines in Fig. 2a& 2b. With an only 2 × 2 pixels detector, ptychography with the reciprocal space upsampling outperforms iDPC with 1.6 times better resolution by comparing the full widths at half maximum (FWHM) – 0.51 vs 0.80 Å. This is also reflected by the depth of dip between the 2 atoms in the 1.36Å dumbbell structure: Ptychography cleanly resolves this dip at almost 100%, which surpasses the 56% dip from iDPC. The scalebar is 2Å and the colorbar is the same for both images.

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