Integrated Differential Phase Contrast (iDPC) STEM: A New Atomic Resolution STEM Technique To Image All Elements Across the Periodic Table

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A new, recently introduced Integrated Differential Phase Contrast (iDPC) STEM imaging technique [1] is enabling live imaging of the phase of the transmission function of thin samples. One of the first striking advantages of this new technique is that it is able to image light (C, O, N …) and heavier elements (Sr, Ti, Ga …) together in one image whereas a standard (HA)ADF-STEM image shows only the heavier atoms. Figure 1 shows an example of SrTiO₃ imaged using the conventional ADF-STEM technique vs. our new iDPC-STEM technique. The oxygen columns and carbon contamination (low frequency information) are clearly visible in the latter and missing in the former.

In order to understand this theoretically we derived mathematical descriptions of the imaging process both for standard STEM techniques (BF, ABF and (HA)ADF) based on ring-shaped detectors [2] and for (i)DPC using a four quadrant (4Q) detector [1]. We found that for any of these STEM techniques the image can be described in Fourier space with

\[ \mathcal{F}\{I_{STEM}\} = CTF_S \cdot \mathcal{F}\{\sin \varphi\} + CTF_C \cdot \mathcal{F}\{1 - \cos \varphi\} \]

where \( \varphi \) is the phase of the transmission function of the sample and \( \mathcal{F} \) denotes Fourier transform. The contrast transfer functions \( CTF_S \) and \( CTF_C \) depend on the probe and the shape of the detector and their full expressions can be found in [2]. This equation is valid for thin samples and for high resolution STEM.

In this nonlinear equation we recognize two “objects” which are \( \sin \varphi \) and \( 1 - \cos \varphi \), respectively. This equation reduces to a linear form for (HA)ADF, as \( CTF_S = 0 \) in this case. The resulting CTF for (HA)ADF is just \( CTF_{ADF} \sim \mathcal{F}\{|\psi_{in}|^2\} \), where \( \psi_{in} \) denotes the probe (see [2]). To lowest order in \( \varphi \) the object is \( 1 - \cos \varphi \approx \varphi^2 \), i.e. ADF images the square of the phase of the transmission function of the sample, which accounts for its difficulty in imaging light elements together with heavy ones.

Standard DPC images are formed by subtraction of the images given by opposite quadrants of the 4Q detector. Using our compact model we can directly analyze the DPC images as it is valid for any (combination of) detector segment(s). This analysis shows that the DPC images are a very good approximation of the components of the center of mass (COM) movement of the CBED pattern for each probe position. Furthermore, as the COM vector of the electron wave intensity is linearly related to the gradient of the phase of the transmission function of the sample, 2D integration of the COM vector image (and also the DPC vector image), resulting in iDPC image, therefore directly yields the phase [1]:

\[ \mathcal{F}\{I_{iDPC}\} \approx \mathcal{F}\{I_{iCOM}\} = \frac{1}{2\pi} \mathcal{F}\{|\psi_{in}|^2\} \cdot \mathcal{F}\{\varphi\} \]

Here \( CTF_{iDPC} \approx CTF_{iCOM} = \frac{1}{2\pi} \mathcal{F}\{|\psi_{in}|^2\} \) and the object is simply \( \varphi \), i.e. the phase of the transmission function.
Figure 2 shows simulated ADF- and iDPC-STEM images using an artificial sample including all atoms from the periodic table (potentials taken from [3]). This clearly demonstrates which atoms can be seen together in one image with each method. As iDPC-STEM directly images the sample potential whereas ADF-STEM images its square, a much lower dynamic range as well as a much lower dose is needed to image light elements like O together with heavier elements like Sr and Ti.

References:


Figure 1. ADF-STEM image (left) and iDPC-STEM image (right) of SrTiO₃ recorded under the same conditions (same area) on a probe corrected FEI Titan Themis machine at 300 kV. Opening angle of the beam was 17 mrad and the field of view 6.5 nm.

Figure 2. Simulated ADF-STEM image (left) and iDPC-STEM image (right) of the periodic table of elements. Atomic potentials were taken from [3]. All rows of the periodic table are visible (including hints of H and He) in iDPC-STEM while ADF-STEM shows elements from the 3th row on (no oxygen).