Quantitative High-Resolution TEM/STEM and Diffraction

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Averaging scheme for the reconstruction of atomic resolution off-axis electron hologram

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For quantitative atomic resolution electron microcopy, the access to the amplitude and phase of the object exit wave is indispensable, as object information is distributed into both channels. Furthermore, the inevitable residual aberrations must be numerically corrected for comparison with calculations as the accuracy of hardware-correctors is limited. A numerical correction requires both amplitude and phase of the electron wave, but conventional high-resolution transmission electron microscopy only offers the access to the amplitude of the image wave, which contains somewhat intertwined amplitude and phase information as given by the transfer function of the microscope.

Several routes exist to achieve access to both the amplitude and phase [1]. A very intriguing one is off-axis holography as the recorded information in the hologram as well as the reconstruction scheme are linear, thus allow a rather straight-forward unbiased access to the exit wave.

As with nearly all electron microscopic techniques, the precision of the obtained information is limited by the number of electrons recorded. For non-beam sensitive materials, this limitation can in principle easily be overcome by longer exposure times. However, the limited temporal stability of the instrumentation prohibits extended exposures, as for instance the specimen or biprism start to drift.

This limitation can be overcome in principle by compensating the instrumental instabilities. Such a compensation can be achieved easily by a posteriori off-line processing [2]. We present an electron holographic reconstruction scheme suitable for holograms of atomic resolution. It is based on a series of several holograms (20-30) recorded with exposure times within the stability limits of the instrument (2-8s). The object holograms are recorded using a double biprism setup in order to reduce diffraction artifacts [3, 4] and due to the improved experimental flexibility [5]. The complex wave functions of these holograms are off-line processed in two steps. In a first step, a common region of interest is selected across the series while compensating coarse drift via central band cross-correlation. In the second step the side-bands of these regions are reconstructed and the resultant wave functions are preliminarily averaged, while compensating subpixel specimen drift, defocus drift (corresponds to specimen Z-drift), biprism drifts as-well-as hologram contrast variations. Between the iterations the individual drifts are estimated based on the preliminary average and the averaging/estimations are repeated iteratively until the averaged wave converges (Fig. 1).
Figure 2 show the phase and amplitude exit wave of a GaAs wedge reconstructed from 20 holograms of 2 second exposure time. The wave was corrected for residual aberrations using the edge on the lower right as reference. The stronger phase shifts of the heavier As-columns compared to the Ga-columns can be easily identified in the thicker region at the top of the exit wave.

In the vacuum region the standard deviations of the phase and amplitude are 2π/104 and 0.04. At this precision the uncertainty in the residual aberrations and in residual specimen tilt, as-well-as the changes of the specimen structure (especial of the amorphous surfaces and the enhanced vibration of the edge atoms) are the next obstacles to overcome for true matching of the experimentally obtained exit wave-function with simulated ones.

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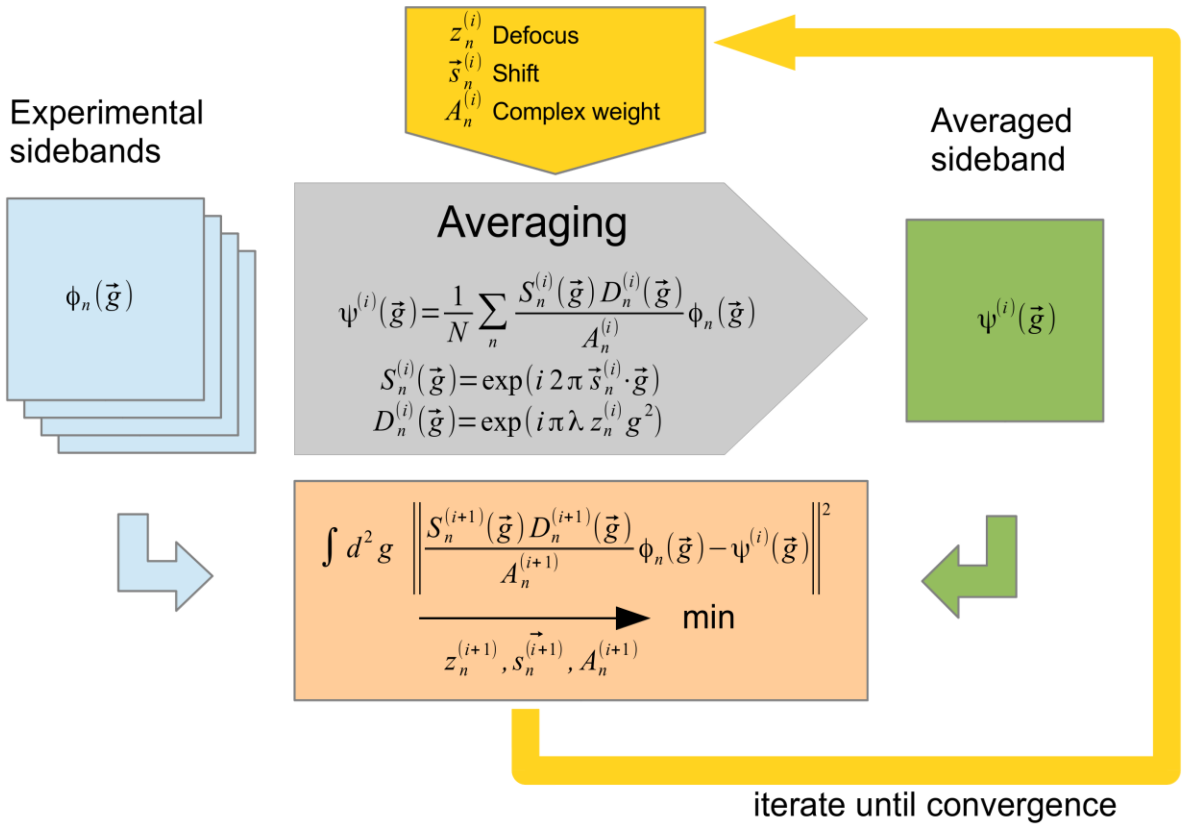

Figure 1. Algorithm for adjustment of the parameters for defocus, shift and global phase and amplitude: For each experimental sideband the parameters are optimized with respect to the distance to the averaged sideband. The averaging and optimization are repeated until convergence.

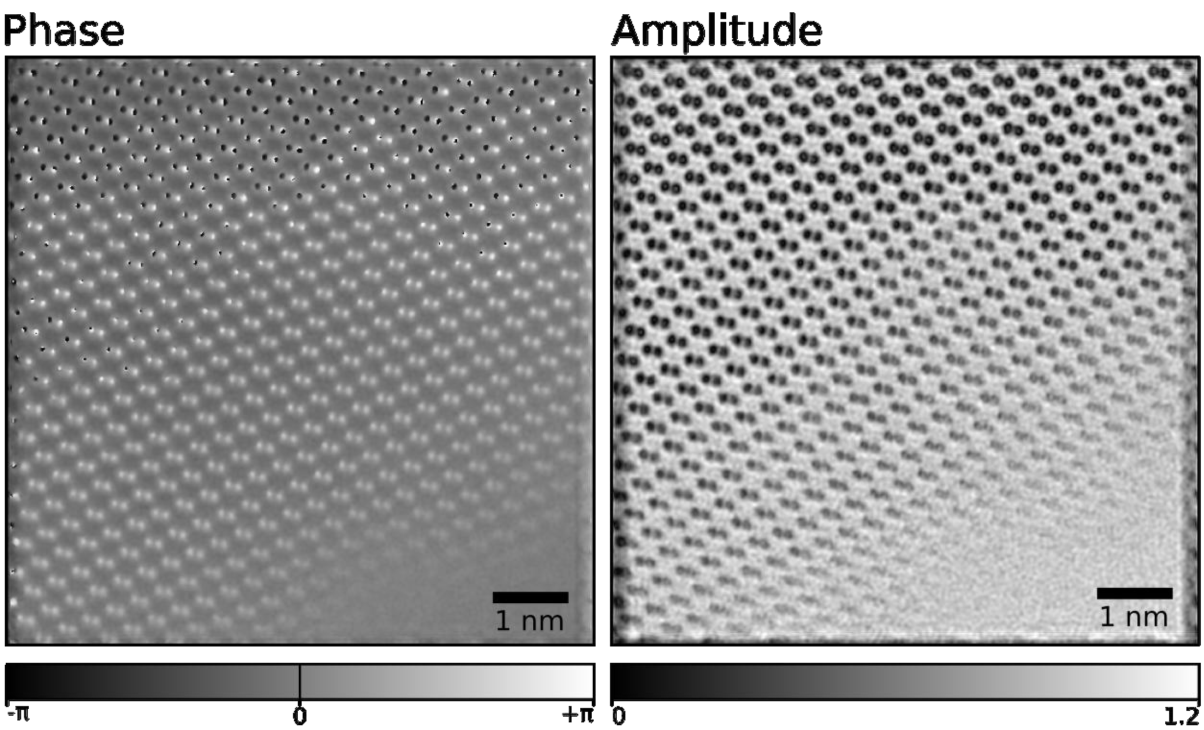

Figure 2. Phase and amplitude of the exit wave of a GaAs wedge after numerical aberration correction. The defocus was corrected for the lower-right edge to the vacuum.