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Comparison of intensity and absolute contrast of simulated and experimental high-resolution transmission electron microscopy images for differerent multislice simulation methods

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In high resolution transmission electron microscopy (HRTEM) a disagreement of absolute contrast between experimental and simulated images has frequently been reported [1-5]. Intensity discrepancies result in a lower value of the dimensionless quantity of image contrast, defined as the standard deviation of image intensity divided by the mean intensity. Simulated contrast values deviated by a factor of more than 3 from experimental ones [1]. This discrepancy, known as the Stobbs factor problem has prevented the evaluation of absolute HRTEM contrast by comparison with simulated data as has been successfully done with high angle annular dark field scanning transmission electron microscopy (HAADF-STEM) [6].

It has been shown that a crucial part of this mismatch is due to not properly considering the influence of the camera used for acquisition expressed by the modulation-transfer function (MTF) [7]. Furthermore, it has been proposed that additional overestimation of contrast in simulations could be attributed to both the usage of absorptive potentials for thermal diffuse scattering (TDS) resulting in a loss of diffuse intensity and to the treatment of spatial incoherence using the coherent envelope approach damping intensity scattered to high angles [8]. A frozen lattice (FL) approximation [9] combined with incoherent summation of intensities simulated for different incident angles that are Gaussian distributed with the semi-convergence angle accounting for spatial incoherence is a more adequate model [9].

The influence of each of these simulation methods on the contrast of HRTEM micrographs was examined by studies of simulated defocus series for different objective apertures. As can be seen in Figure 1 that shows the results for the simulation of 15 nm thick gold viewed along [100] zone axis, the proper use of the MTF yields the largest contrast reduction by a factor of 2.4. The consideration of TDS by the FL model instead of absorptive potentials only yields a small contrast decrease of maximal 1.1. Incoherent summation of different incident angles for the treatment of spatial incoherence contributes another reduction of about 1.2. For larger objective apertures, the use of the coherent envelope approach instead of the more accurate transmission cross coefficients (TCC) also causes overestimation of image contrast, as damping of high-angle scattered intensity has more impact here.

The mismatch of experimental micrographs and simulations, conducted with the FL method, incoherent summation and properly considered MTF, was investigated. For that purpose, the MTF was measured and used in the simulations. Defocus series of a gold foil oriented in [100] zone axis were acquired with a C_S-corrected microscope. Specimen thickness and orientation were determined by parallel beam electron diffraction refinements and the FL simulations were conducted for these parameters and the measured residual spherical aberration.

With a small objective aperture of 7 nm^{-1} radius, a very good agreement is achieved between simulation and experiment qualitatively for the images and quantitatively for the intensities measured in units of incident intensity. The image contrast also coincides, which is shown in Figure 2. The ratio of simulated and measured contrast is 0.98±0.07.

For larger objective apertures a contrast discrepancy of 1.2 is found and a good agreement of intensities is observed. Without any aperture the difference of contrast amounts to a factor of 1.4; this is still smaller than previously reported values of more than 3.

The contrast mismatch between HRTEM simulations and experiments is definitely reduced by proper consideration of the camera MTF and FL simulations with incoherent summation but still remains observable especially with larger or no apertures applied in the imaging process.

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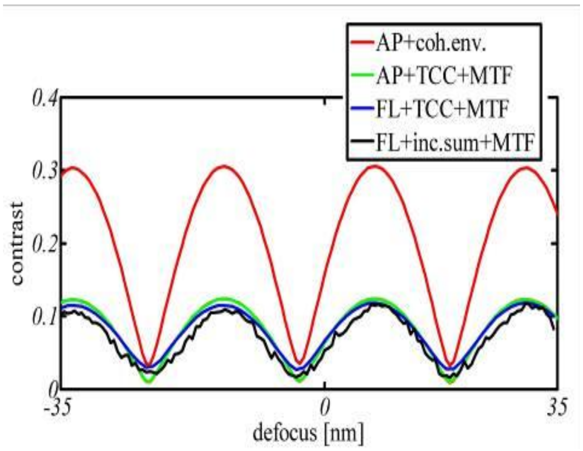

Figure 1: Contrast of images of a defocus series simulated for 15 nm gold in [100] direction with different techniques with an objective aperture of radius 7 nm^{-1}: The red curve is the result of conventional MS calculations and incoherence treated by the coherent envelope approach, the application of the MTF yields the green curve that. For the blue was simulated with incoherent summation.

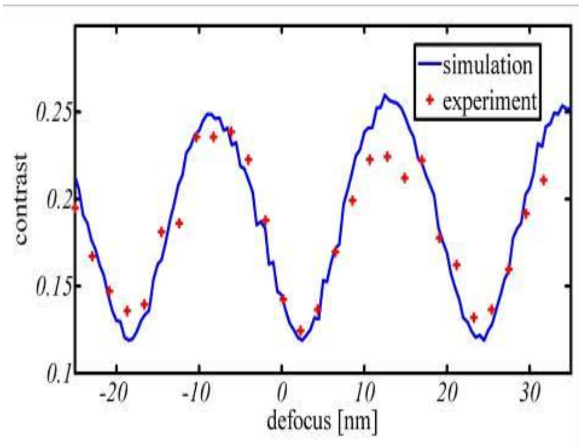

Figure 2: Comparison of experimental and simulated contrast of a defocus series of [100] oriented gold of 12 nm thickness and an objective aperture of 7 nm^{-1} radius. Both the values and the periodicity agree wellof absorptive potentials. For the black curve additionally FL simulations were used instead onein addition to that incoherence was also calculated with TCC instead