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IT-2-P-2322 Comparison of intensity and absolute contrast of simulated and experimental high-resolution transmission electron microscopy images for different multislice simulation methods

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Discrepancies between experimental and simulated images were often reported for high resolution transmission electron microscopy (HRTEM). Simulated contrasts deviate by a factor of up to 3 from experimental ones [1,2]. This disagreement, termed Stobbs factor, has prevented evaluation of HRTEM contrast by comparison to simulations as successfully realised in Z-contrast scanning TEM [3]. The mismatch is caused mainly by improper consideration of the camera modulation-transfer function (MTF) [4]. It was further proposed that contrast-overestimation could be attributed to the use of absorptive potentials (AP) for thermal diffuse scattering (TDS) and to the treatment of incoherence by coherent envelopes [5]. A frozen lattice (FL) simulation with incoherent summation of intensities simulated for various Gaussian-distributed incident angles is more adequate.

The influence of each of these simulation methods on HRTEM contrast was examined by studies of simulated defocus series. Figure 1 shows the results for the simulation of 15 nm thick gold, the proper use of the MTF yields the largest contrast reduction by a factor of 140%. The consideration of TDS by FL instead of AP yields a small contrast decrease below 10%. Incoherent summation of different incident angles contributes a reduction of about 20%. Use of the coherent envelopes instead of the more accurate transmission cross coefficients (TCC) also causes overestimation of image contrast of 10%.

The mismatch of experiments and simulations, conducted with FL, incoherent summation and properly considered MTF, was investigated. Defocus series of a gold foil were acquired with a CS-corrected microscope. Specimen thickness and orientation were determined by diffraction pattern refinements and FL simulations were conducted for these parameters. With an aperture of 7 nm-1 radius, a very good agreement is achieved for image patterns and intensities quantitatively measured in units of incident intensity. The image contrast also coincides as shown in Fig. 2. The ratio of simulated and measured contrast is 0.98 ± 0.07. For larger apertures a discrepancy of 20% is found and good agreement of intensities is observed. Without any aperture the difference amounts to a factor of 40%. Residual aberrations and drift as cause for this were ruled out.

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 with larger apertures.

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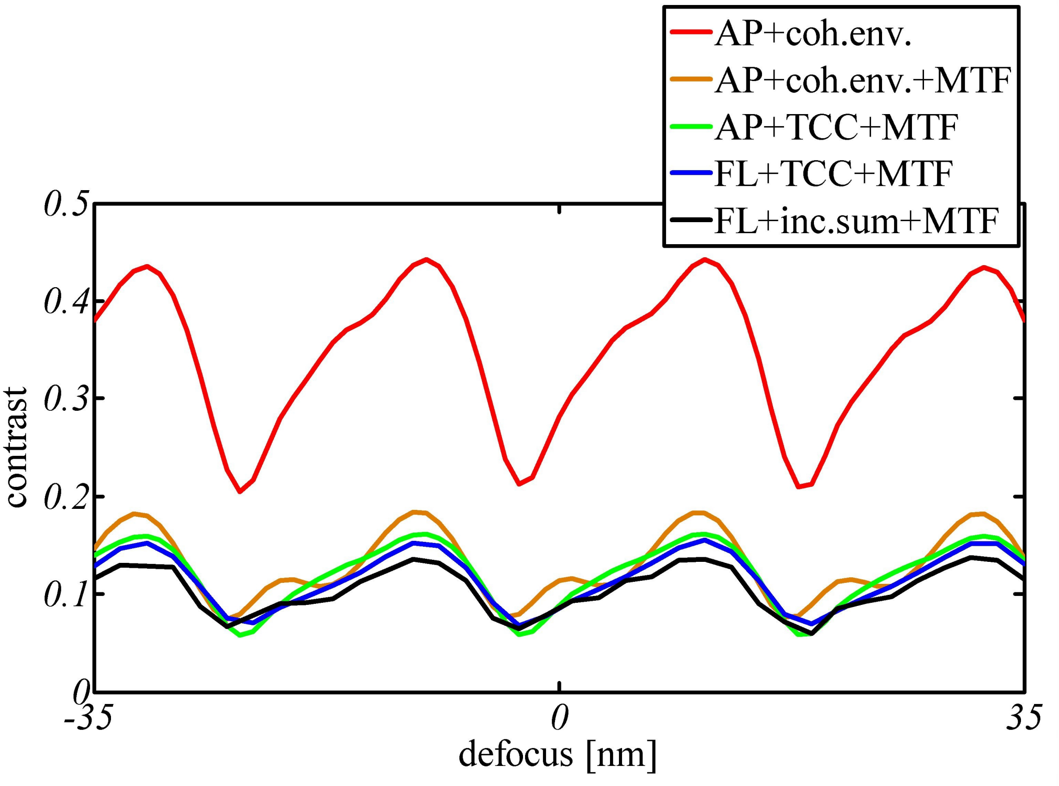

Fig. 1: Contrast of images of a defocus series simulated for 15 nm gold in [100] direction with different techniques using an objective aperture of radius 14 nm-1: The red curve is the result of conventional MS and incoherence treated by coherent envelopes. For the following curves, the image formation was successively simulated more accurately.

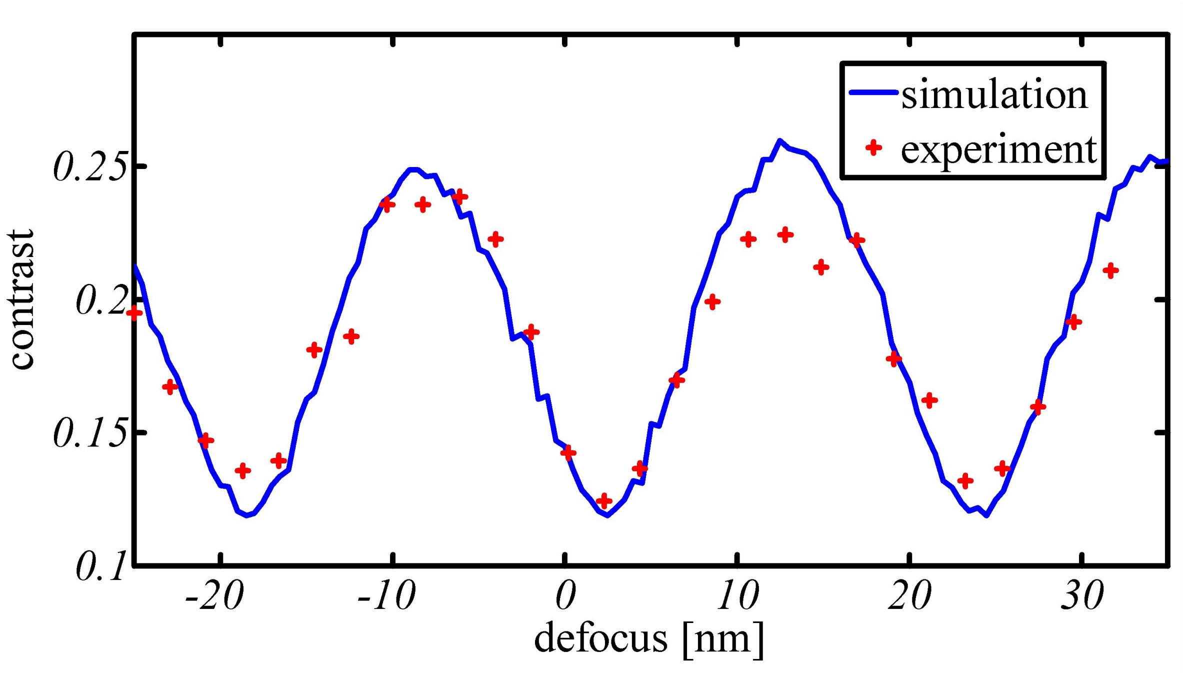

Fig. 2: Comparison of experimental and simulated contrast of a defocus series of [100] oriented gold of 12 nm thickness and an objective aperture of 7 nm-1 radius. Both the values and the periodicity agree well.