Quantitative High-Resolution TEM/STEM and Diffraction

IM.1.P019
Towards an experimental realization of inverse dynamical electron scattering

W. Van den Broek[1], C.T. Koch[1]

[1]Ulm University, Institute of Experimental Physics, Ulm, Germany

wouter.vandenbroek@uni-ulm.de
Keywords: inverse dynamical electron scattering, artificial neural network, atomic resolution tomography

In [1] it is shown that dynamical scattering of fast electrons can be inverted by recasting the multislice algorithm as an artificial neural network [2], enabling the iterative retrieval of the three-dimensional object potential. This allows a non-heuristic treatment of the modulation transfer function of the CCD, partial spatial and temporal coherence and inelastic scattering through an absorptive potential. Furthermore, prior knowledge about the atomic potential shape and the sparseness and positivity of the object can be used. The method is dubbed IDES, inverse dynamical electron scattering.

The backpropagation algorithm [2] calculates the derivative of the error function *E*—the sum of square differences between model and measurements—with respect to the object potential very efficiently in just one extra pass through the network. These derivatives are then used in a type of steepest descent optimization that finds the object in typically ~1000 iterations.

In Ref. [1], IDES was demonstrated on simulated high resolution transmission electron microscope images. The potential of a cuboctahedral Au nanoparticle with 309 atoms arranged in an fcc lattice was reconstructed from 25 noisy images required at a double tilt of −10°, −5°, 0°, 5° and 10° around the two axes. The reconstruction of the potential was faithful; all atoms were reconstructed on the correct positions.

However, in practice the microscope parameters are only known approximately. It is therefore necessary to estimate them simultaneously with the object. In Ref. [3], for example, it is shown that ptychographic reconstructions improve dramatically if the shape and position of the illuminating probe is estimated along with the exit wave. By invoking the chain rule for complex analysis, the error can be derived with respect to the focus value and this derivative can be plugged in the steepest descent optimization. To give priority to the object reconstruction during the first iterations, the derivative is multiplied with $1 - 2^{-n/128}$, with n the iteration number.

In this abstract, a simulation with the same test object as in [1] is performed; see Figure 1. and Table 1. In Figure 2. it is shown that if the initial guess for the focus value of each image is off by a random amount between -5 nm and 5 nm all atom positions can be retrieved if the foci are estimated along with the object. In the other case, a non-physical solution was found. After optimization, the average difference with the real focus values is 0.27 nm (see Figure 3.) and although this value is larger than the slice thickness, no vertical translation of the object is observed.

This work, see [4] as well, paves the way towards an experimental realization of IDES. Apart from focus, also the other microscope parameters, like tilt or residual astigmatism, could be optimized along with the object, as long as sufficiently good starting values are known. [5]

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5. The authors acknowledge the Carl Zeiss Foundation as well as the German Research Foundation (DFG, Grant No. KO 2911/7-1)

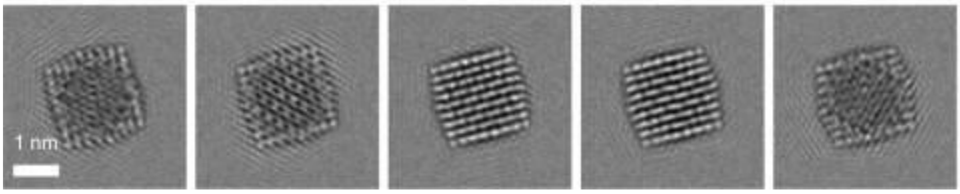

Figure1. Five typical images. From left to right, the tilt is −10°, −5°, 0°, +5° and +10°.

U	C_1	C_3	α	Δf	Δ_{xy}	Δ_z	a	c	d
40 kV	-10 nm	14 μm	0.1 mrad	1 nm	0.025 nm	0.21 nm	0.58	2.7 pix	3.9 pix

Table 1. The simulation parameters. U is the acceleration voltage, C_1 the focus value, C_3 the spherical aberration, α the illumination semi-angle, Δf the focal spread, Δ_{xy} the size of the horizontal dimensions of the voxels, Δ_z the slice thickness, and a, c and d characterize the modulation transfer function [1].

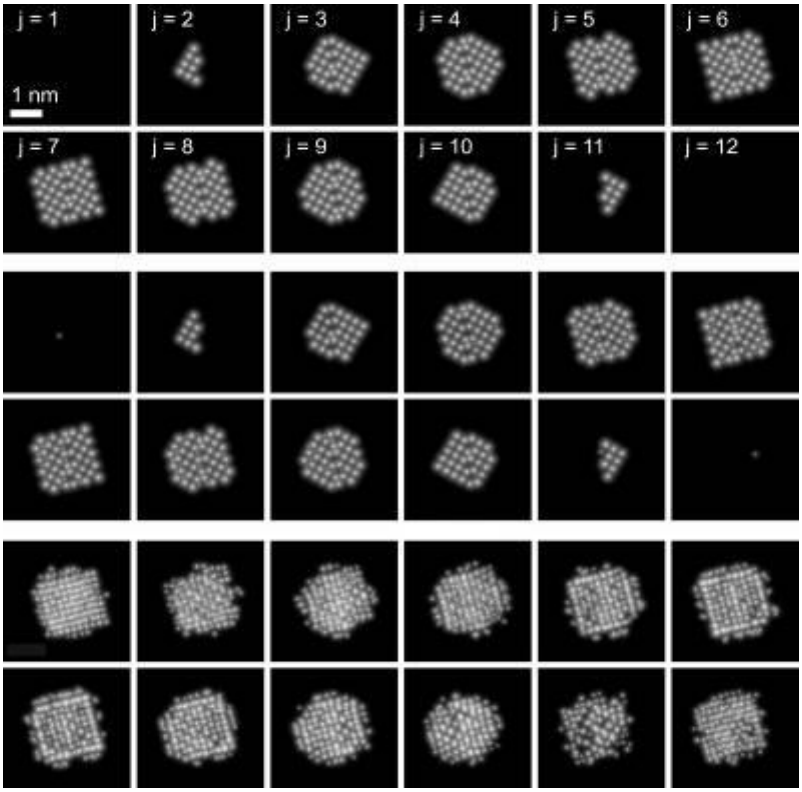

Figure 2. *Upper two rows*: The sliced potential of the test object, on a logarithmic gray scale. *Middle two rows*: Reconstruction with simultaneous defocus estimation. *Lower two rows*: Without defocus estimation.

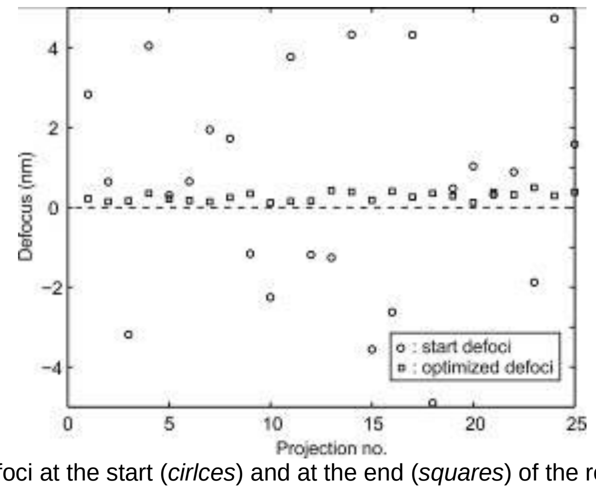

Figure 3. Defoci at the start (*cirlces*) and at the end (*squares*) of the reconstruction.