# Model based tomography in high resolution HAADF STEM

W. Van den Broek[1], S. Van Aert[1], D. Van Dyck[1]

1. EMAT, University of Antwerp, Groenenborgerlaan 171, 2020 Antwerp, Belgium.

wouter.vandenbroek@ua.ac.be
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We present a new reconstruction algorithm for atomic resolution tomography. The projection requirement is fulfilled if the image intensity of multiple atoms is the sum of the image intensities of the individual atoms. This is approximately true in high angle annular dark field scanning transmission electron microscopy (HAADF STEM) [1].

The algebraic reconstruction technique writes the projection process as a matrix product $Wf = P$, where $f$ is the unknown object, $W$ a weight matrix and $P$ the projections. For every pixel $i$ in $P$ and every voxel $j$ in $f$, we define the weight $w_{ij}$ as the value in $i$ of an image of a single atom positioned in $j$, see Fig. 1. The image of an atom is determined by its potential, the probe distribution and the detector geometry, these weights therefore bring prior knowledge in the reconstruction, i.e. make the tomographic algorithm model based. The spatial extent of an atom image is accounted for completely by $W$, the object $f$ therefore only consists of Dirac functions on the atom positions and zeros in between.

Usually reconstruction algorithms calculate 2D images only, and do 3D reconstructions by treating the object as a stack of 2D slices. This is impossible in our case because the image of the atom extends in the two dimensions normal to the beam direction. Therefore a MATLAB program was written that reconstructs the 3D object directly out of the 2D projections.

The object $f$ is found by maximizing the likelihood that the projections $Q$ measured with Poisson noise are brought forth by the object $f$. The iterative algorithm accomplishing this is: $f^{k+1} = f^k W^T Q / (Wf^k)$, where arithmetic operations between vectors are elementwise and $W$ is normalized such that each column sum is 1 [2]. $f$ is composed of Dirac functions separated by the vacuum, so every voxel with a value below half of the average of the non-zero voxels is likely to lay in the vacuum. Hence we set its value to zero and compensate for the loss in intensity by multiplying the values of the non-zero voxels with a constant. This is repeated for every iteration $k$. This greatly accelerates convergence.

We did a simulation of an amorphous silicon (Si) particle consisting of 43 atoms. The image of a Si atom was calculated with STEMsim [3] under Scherzer conditions for a spherical aberration of 0.5 mm, a high tension of 300 kV and a detector ranging from 60 to 100 mrad. There were 36 projections with a 4° interval and a missing wedge of 40°. Poisson noise degraded the mean signal-to-noise ratio of the non-zero pixels in $P$ to the low value of 3. In Fig. 2 a top view of the object $f$ is shown, and in Fig. 3 we see the noise-free projection of 88°. The voxels and pixels are 0.3 Å wide. The algorithm converged before the 512$^{th}$ iteration, as evidenced by the fact that $f^{512}$ equals $f^{1024}$ exactly. In Fig. 4 the same top view of the reconstruction as in Fig. 2 is given, for every voxel we found out exactly if it contains an atom or not. The values of the voxels with atoms are distributed around 136.5 with a standard deviation of 3.9 counts.

To our knowledge, this is the first reconstruction algorithm that takes into account the atomic nature of the object, the form of the atomic potential and the probe, and the detector geometry. This makes the result less sensitive to the high level of noise, the high angular increment between projections and the large missing wedge. Since the algorithm converges, no arbitrary stopping criterion is needed and we have a true maximum likelihood estimator of the object. [4]


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1. P. Hartel et al., Ultram. **63** (1996) p93.
2. F. Natterer, et al. Mathematical Methods in Image Reconstruction, SIAM, Philadelphia, 2001.
3. A. Rosenauer, et al., Springer proceedings in physics: microcopy of semiconducting materials (MSM) Conference 2007, Cambridge.


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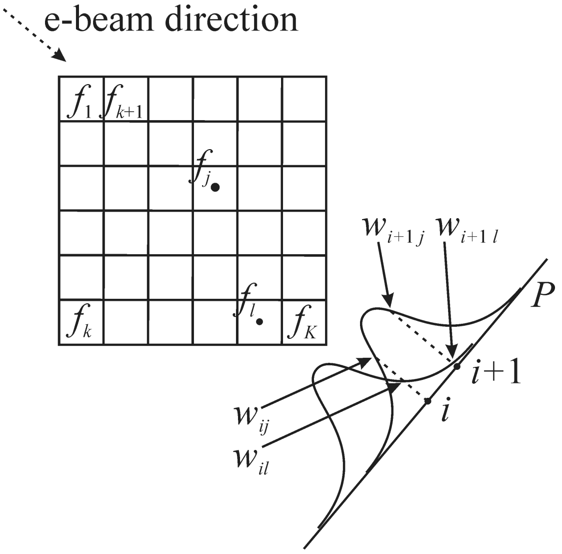


**Figure 1.** The atom in position $j$ gives rise to the right intensity profile, the atom in position $l$ to the left profile. The resulting image $P_i$ in $i$ is the sum of the values in $i$ of both profiles, i.e. $P_i = w_{ij}f_j + w_{il}f_l$.

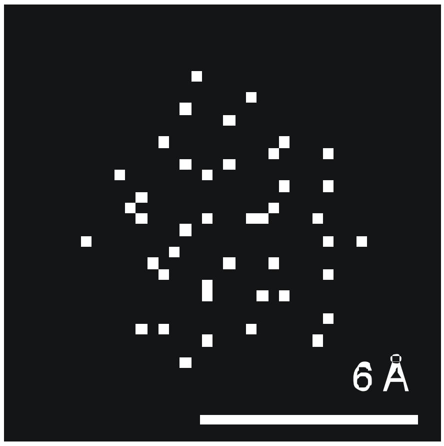


**Figure 2.** Top view of the object $f$, a Si particle, corresponding to approx. the same angle as in Fig. 3.

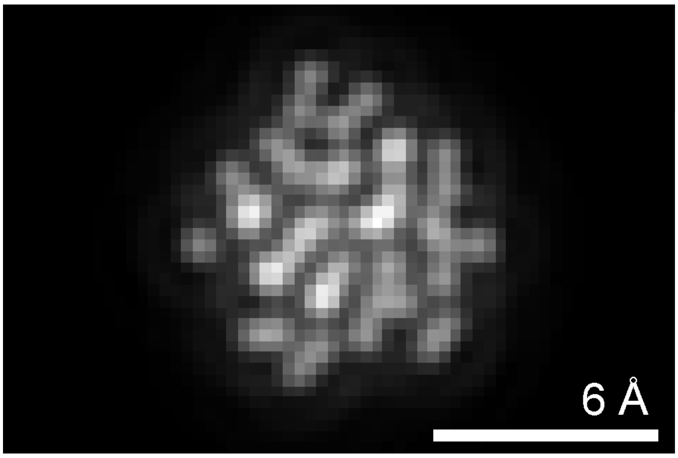


**Figure 3.** The projection $P$ obtained by multiplying $f$ with the weights $W$ for an angle of 88°.

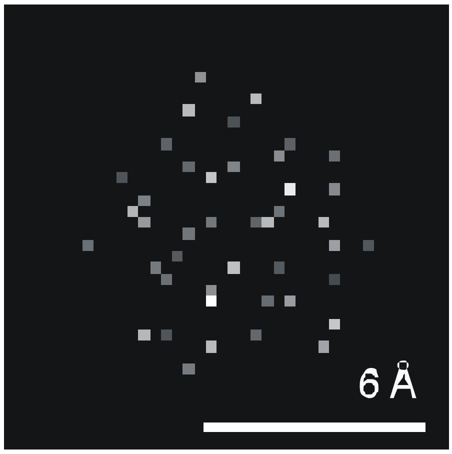


**Figure 4.** Top view of the reconstruction. The contrast is adjusted to show the variance in the values of the non-zero voxels.

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