Towards electron holography of 3D magnetization distributions in nanoscale materials using a model-based iterative reconstruction technique

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Simulation of phase maps (forward model)

The magnetic phase shift originating from a magnetic specimen examined in the TEM can be described in terms of the Aharanov-Bohm effect:

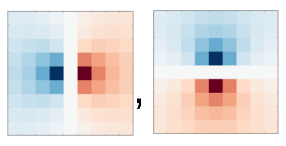
$$\varphi_m(x,y) = -\frac{\pi}{\phi_0}\int A_z(x,y,z)\,dz \quad \text{with} \quad \boldsymbol{A}(\boldsymbol{r}) = \frac{\mu_0}{4\pi}\int \boldsymbol{M}(\boldsymbol{r}')\times\frac{\boldsymbol{r}-\boldsymbol{r}'}{|\boldsymbol{r}-\boldsymbol{r}'|^3}\,d\boldsymbol{r}'$$

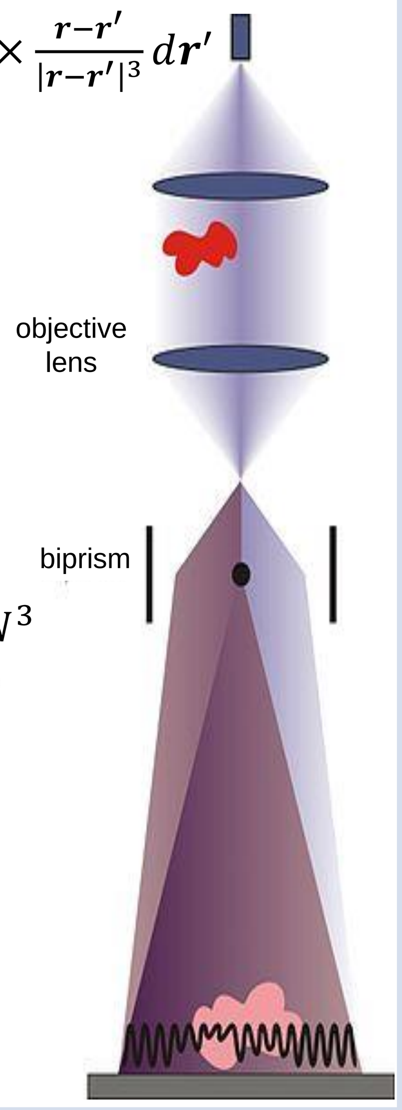
$$\Rightarrow \varphi_m(x,y) = -\frac{\mu_0}{4\phi_0}\int\int\frac{(y-y')M_x(\boldsymbol{r}')-(x-x')M_y(\boldsymbol{r}')}{|\boldsymbol{r}-\boldsymbol{r}'|^3}\,d\boldsymbol{r}'\,dz$$

Forward Model as a (linear) matrix operation:

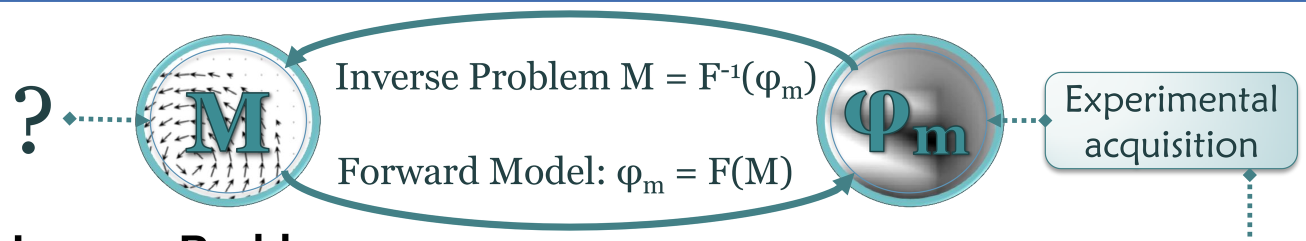
$$\boldsymbol{y} = \boldsymbol{F}(\boldsymbol{x}) = \mathbf{F}\cdot\boldsymbol{x} = \mathbf{Q}\cdot\mathbf{P}\cdot\boldsymbol{x}$$

- $\boldsymbol{y}$: vectorized phase information → N^2
- $\boldsymbol{x}$: vectorized magnetization distribution → $3N^3$
- $\mathbf{F}$: matrix of the complete forward model → $N^2 \times 3N^3$
  - $\mathbf{P}$: projection matrix → $2N^2 \times 3N^3$ (sparse)
    →Use dedicated sparse matrix libraries
  - $\mathbf{Q}$: phasemapping matrix → $N^2 \times 2N^2$ (dense)
    →Few unique entries, use lookup tables of the kernels for intelligent multiplications

conv. kernels:  $\propto \frac{1}{r^2}$



Model-based iterative reconstruction technique

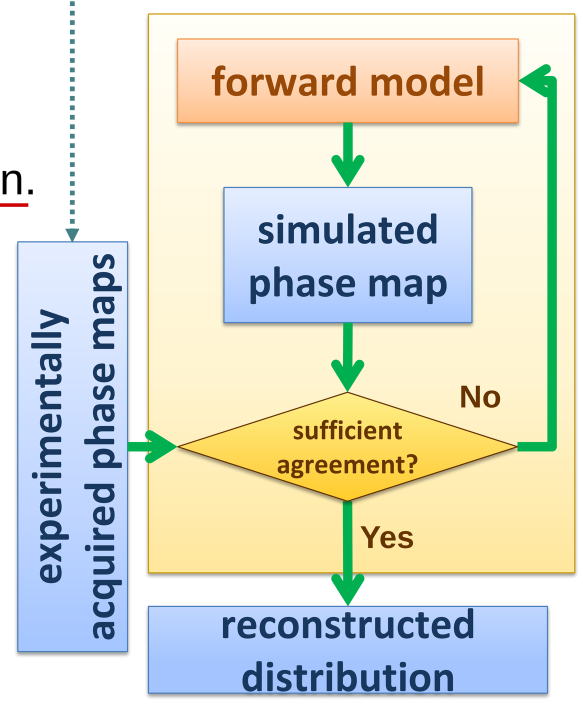


Inverse Problem:
Retrieve the magnetization distribution from a given set of phase maps via a model-based reconstruction algorithm.
→ ill posed problem → non-unique solution → regularization.

Minimize the cost function:

$$J(\boldsymbol{x}) = \|\boldsymbol{F}(\boldsymbol{x})-\boldsymbol{y}\|^2_{\mathbf{S}_\epsilon^{-1}} + \lambda\|\boldsymbol{x}\|^2_{\mathbf{S}_a^{-1}}$$
$$= (\boldsymbol{F}(\boldsymbol{x})-\boldsymbol{y})^T\mathbf{S}_\epsilon^{-1}(\boldsymbol{F}(\boldsymbol{x})-\boldsymbol{y}) + \lambda\boldsymbol{x}^T\mathbf{S}_a^{-1}\boldsymbol{x}$$

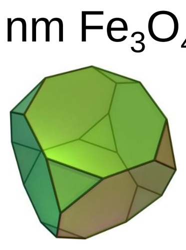
- $\mathbf{S}_\epsilon$: covariance matrix of the measurement errors
- $\mathbf{S}_a$: a priori covariance of the magnetization distribution
- λ: regularization parameter.



Regularization selects the most physical solution from the pool of possible solutions by including physical constraints.
→ Minimize magnetic exchange energy : $E_{ex} = A\int_V\left((\nabla M_x)^2 + (\nabla M_y)^2 + (\nabla M_z)^2\right)dV$
(Corresponds to first-order Tikhonov regularization; favors slow variations in $\boldsymbol{M}$).

Reconstruction of projected magnetization distributions from experimental phase maps

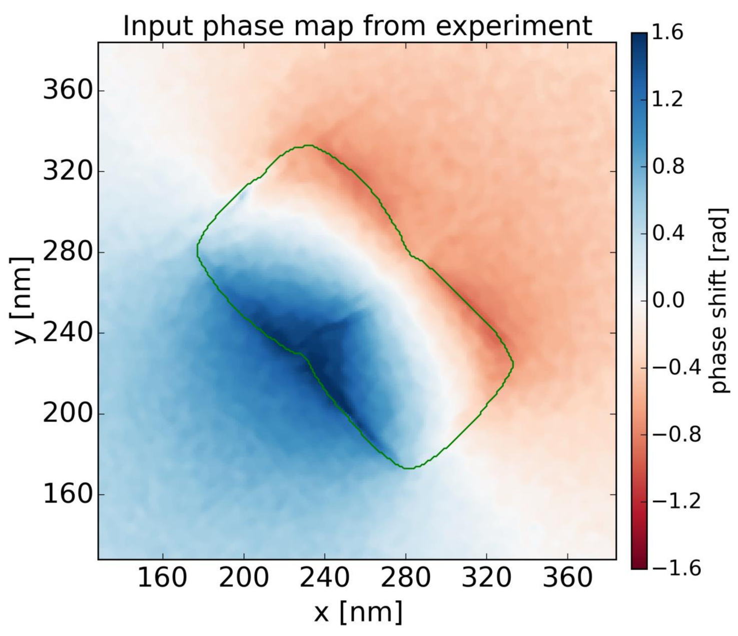
Test Case:
Array of ~50 nm Fe_3O_4 nanocubes.



Goal:
Retrieve the projected (in-plane) magnetization inside the particles from one experimentally acquired phase map. Use masks to determine the particle positions.

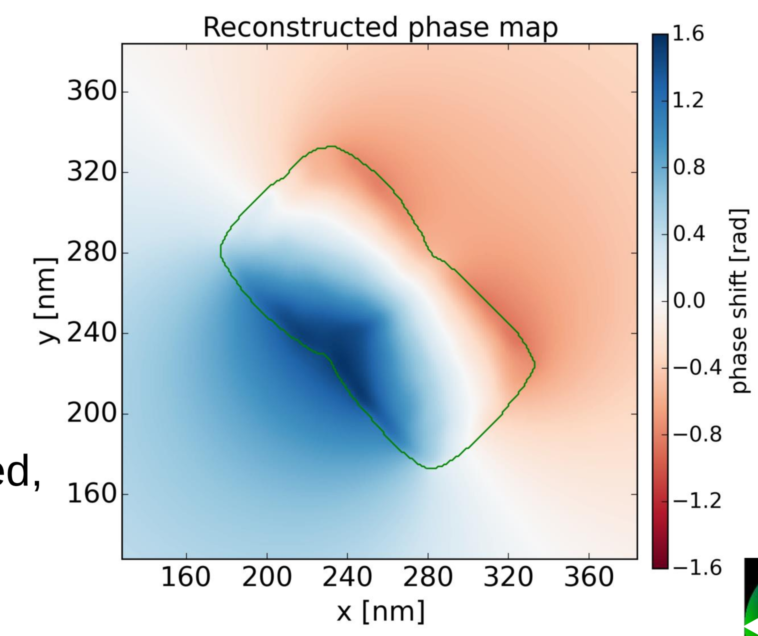
Result:
Reconstructed distributions show distinct projected magnetization structures (homogeneous and vortex states).
Phase maps from reconstruction are compared to input in the figures to the right.
RMS deviation:
→ 2 particles: 0.042 rad
→ 4 particles: 0.064 rad

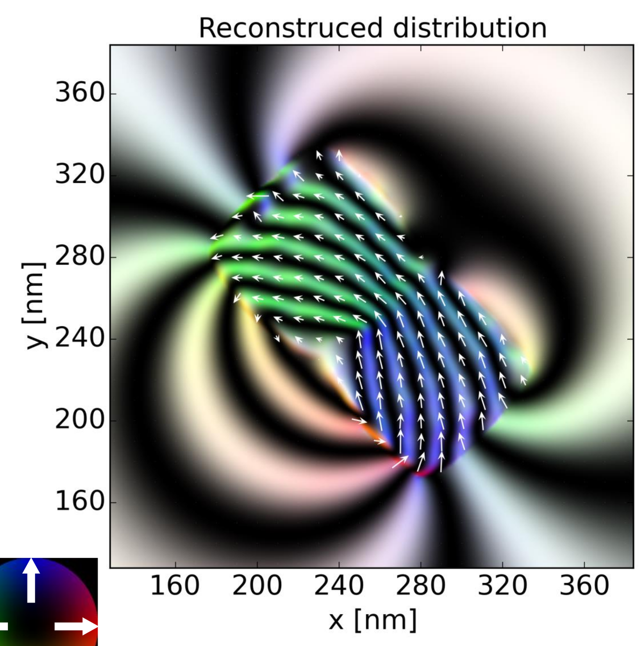
Experimentally acquired single phase map as input | Best-fitting phase map generated from reconstructed distribution | Reconstructed distribution with superimposed contour map

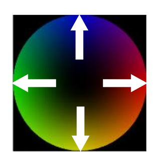


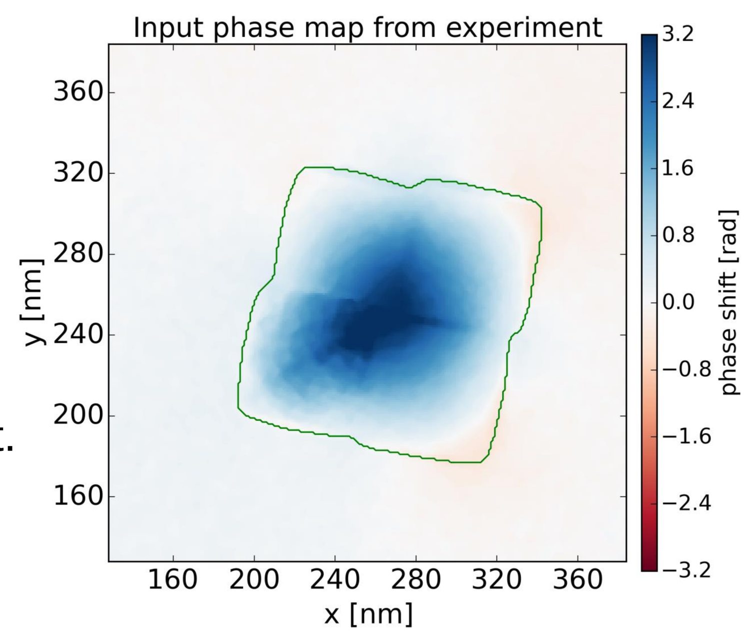
Reconstruction

Array of 2 particles, each homogeneously magnetized, angled roughly at 45°



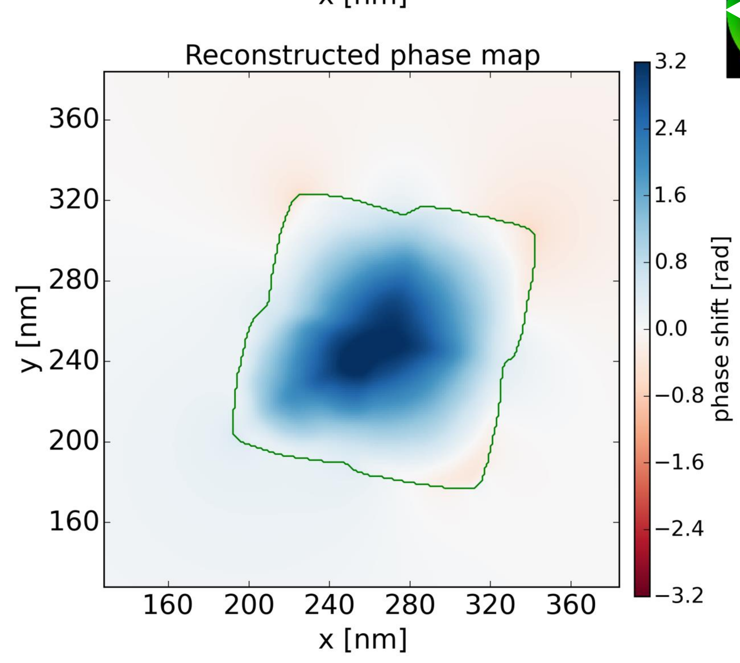


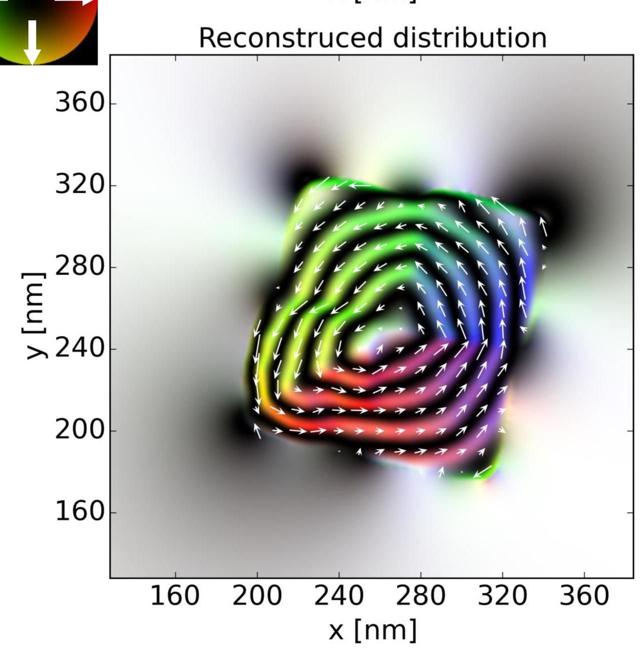




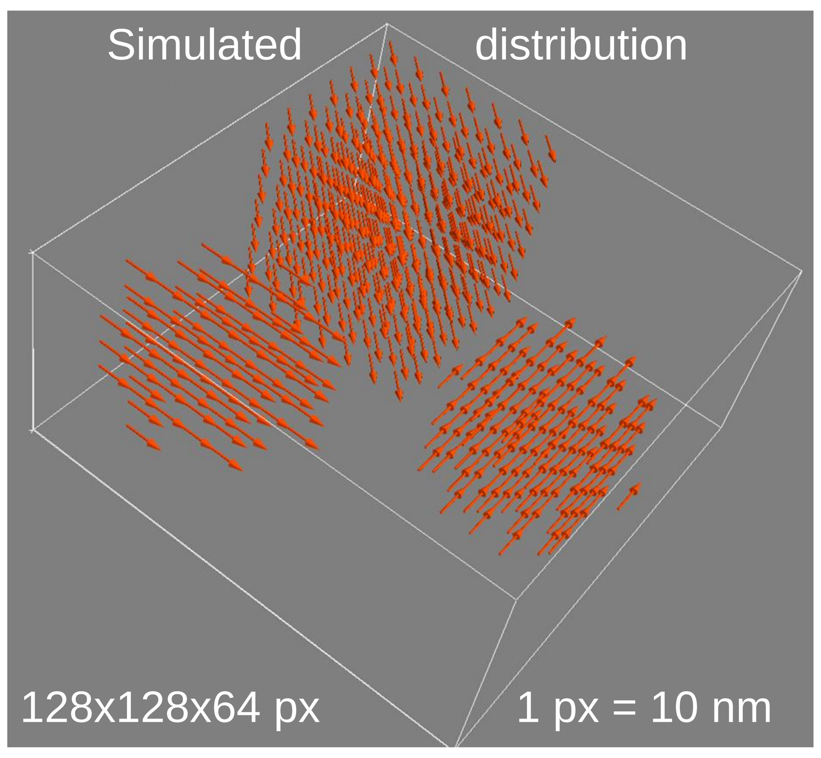
Array of 4 particles, magnetized in an anti-clockwise vortex state

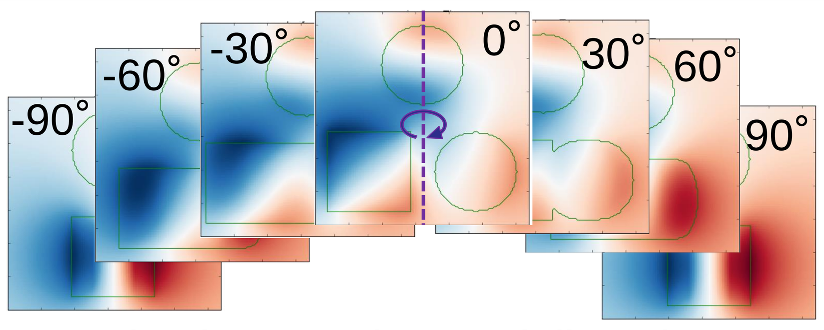
Reconstruction



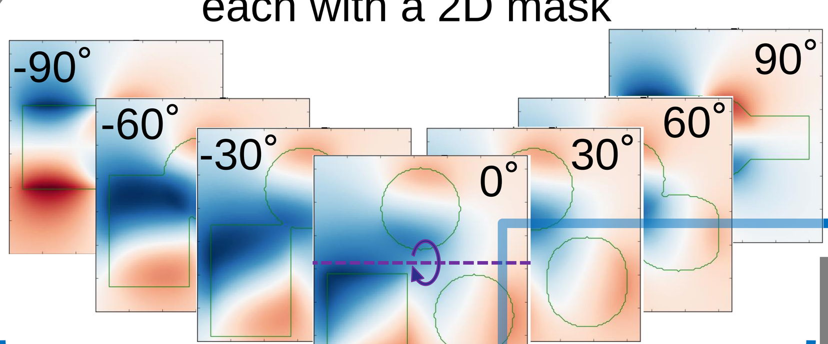


Outlook to the retrieval of 3-dimensional magnetization distributions

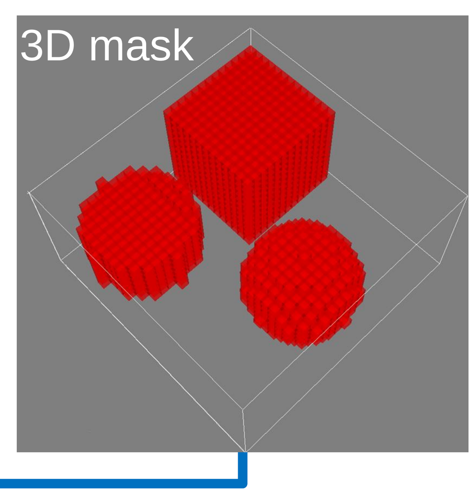




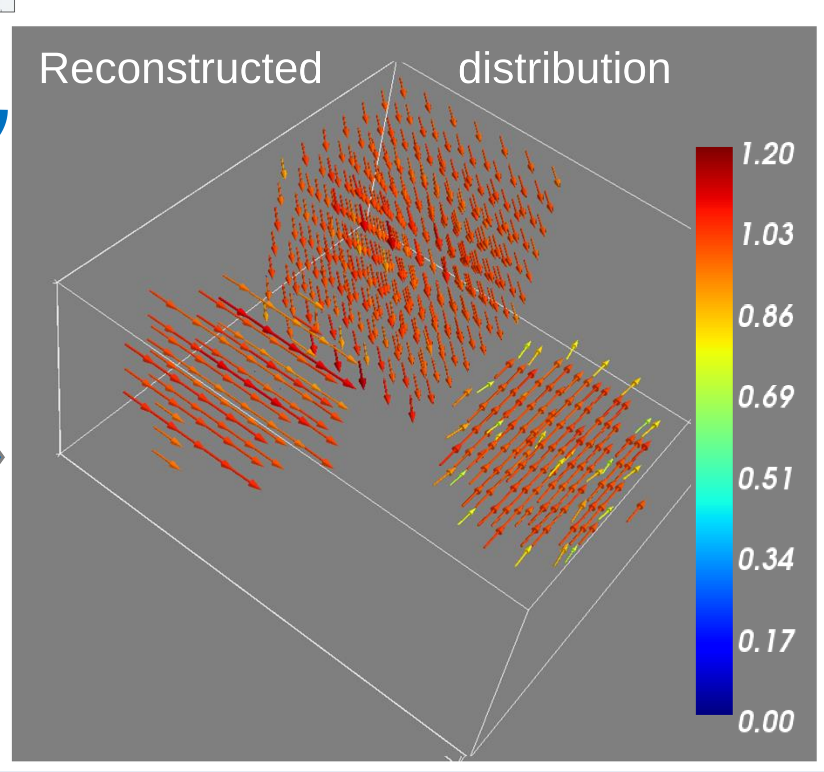
Simulate 2 orthogonal tilt series each with a 2D mask



Determine 3-dimensional mask (backprojection w. transp. matrix)



PYthon based **R**econstruction **A**lgorithm for **M**agnet**i**c **D**istributions



The reconstruction algorithm was tested using simulated datasets for 3D magnetization distributions.
Shown: Array of three homogeneously magnetized objects (slab, disc, sphere).
→ 2 tilt series of 7 projections (orthogonal axes were used as input for the algorithm.

A complete software package is in development.

The model-based approach avoids the artifacts of classical tomographic approaches such as filtered back-projection [3-5].

References

1) Y. Aharonov and D. Bohm, Physical Review, 1959, 115 (3), pp. 485 -491, doi:10.1103/PhysRev.115.485
2) A. Tonomura, Electron holography, Springer Berlin, 1999, ISBN:978-3-540-64555-9
3) C. Phatak et al., Ultramicroscopy, 2008, 108 (6), pp. 503-513, doi:10.1016/j.ultramic.2007.08.002
4) A. Lubk et al., Applied Physics Letters, 2014, 105 (17), doi:10.1063/1.4900826
5) T. Tanigaki et al., Nano letters, 2015, 15 (2), pp. 1309-1314, doi:10.1021/nl504473a

Samples were provided by Alexandra Terwey.

Experimental electron holograms were recorded on an FEI Titan 80-300.

All software is written in the Python programming language using the Python(x,y) distribution for Windows.

Convolutions are implemented using the FFTW library.