Introduction to QSTEM, a quantitative STEM simulation software

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Simulating quantitative STEM (QSTEM) images

Things I considered important when writing QSTEM:

- Potential slicing should work for arbitrary samples (e.g. interfaces, defects, … not just perfect crystals in zone axis)
- It should be possible to compute images for arbitrary orientations, not just low-index zone axes of single crystals
- Atomic scattering factors should be accurate up to the large angles needed for STEM simulations.
- The simulation should be QUANTITATIVE
- Accuracy over speed, but still try to be as fast as possible
- Allow very large simulations to be run on any computer

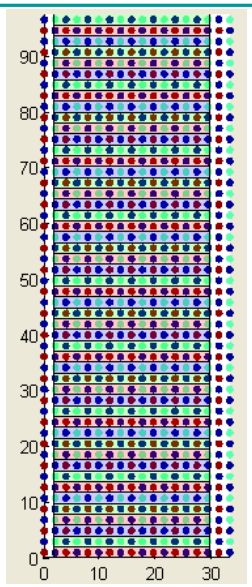
Tilting the sample

$SrTiO_3$

t = 98Å

θ_y **= 0°**

dz = 0.98Å



$SrTiO_3$

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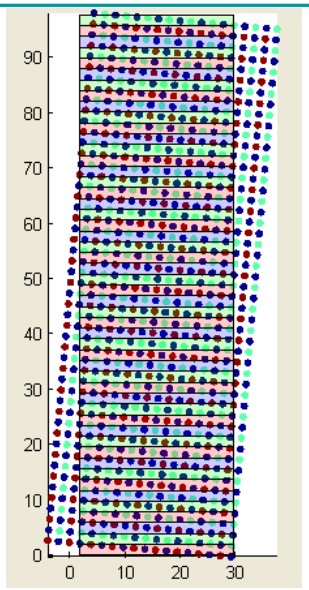
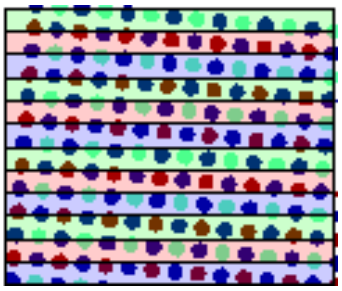


Slice shifting



?

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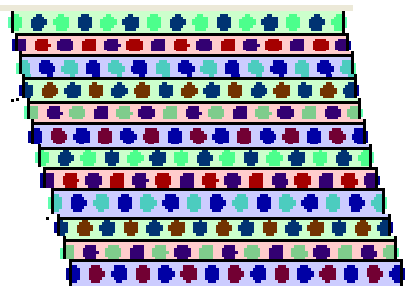
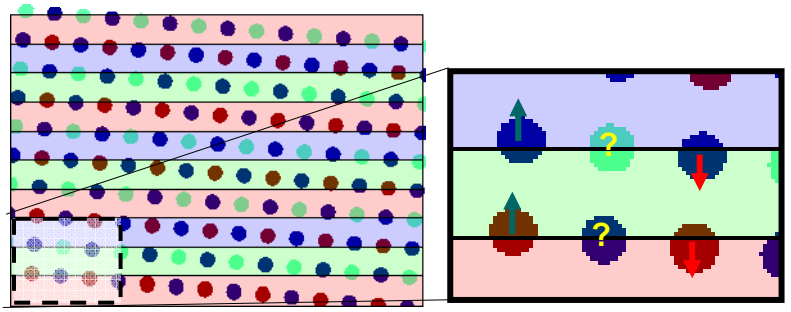


Crystal tilted 5°

Commonly used approximation:
Slice shifting
(This should only be used for very small tilts)

QSTEM does not use slice shifting

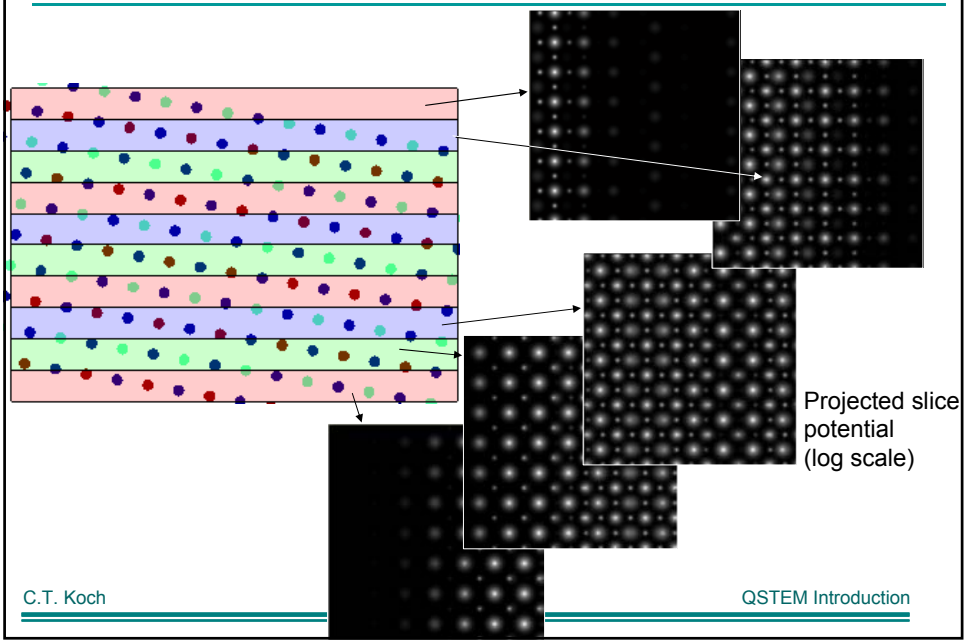
3D slicing of model potential



Problem: To which slice do we assign the atomic projected potential ?

Solution: 1. Compute the 3D potential of the whole model on a fine grid.
2. Slice the 3D potential and integrate potential within each slice.

Potential slices of a tilted specimen



Scattering factors

Acta Cryst. (1994). **A50**, 481–497

Dirac–Fock Calculations of X-ray Scattering Factors and Contributions to the Mean Inner Potential for Electron Scattering

BY DAVID REZ

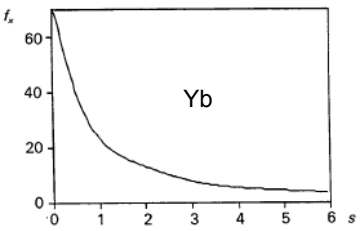
Pennine House, Pennine Drive, London NW2 1PA, England

PETER REZ

Department of Physics and Center for Solid State Science, Arizona State University, Tempe, AZ 85287-1704, USA

AND IAN GRANT

Mathematical Institute, 24/29 St Giles, Oxford OX1 3LB, England



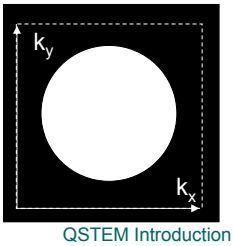
Non-parameterized scattering factors by Rez, Rez and Grant (1994) are being used.

These are tabulated up to $s=\sin(\theta)/\lambda = 6.0$

Avoiding aliasing

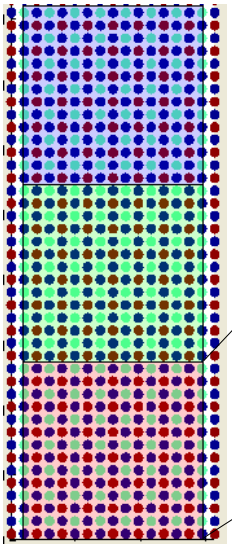
Aliasing artifacts may occur, when numerical operations on an image (or a complex wave function) are performed in reciprocal space. These effects are avoided by

1. Using bandwidth limited lookup tables for the 3-dimensional atomic potential when constructing the slices of the projected potential (no time-consuming bandwidth limiting of the final slices needs to be performed then)
2. The outer 1/3 of the wave function in k-space is set to zero after every Fresnel propagation.

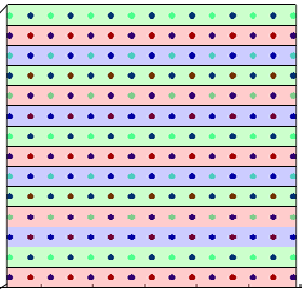


Computing images of large structures

1. Partition the structure in sub-slabs

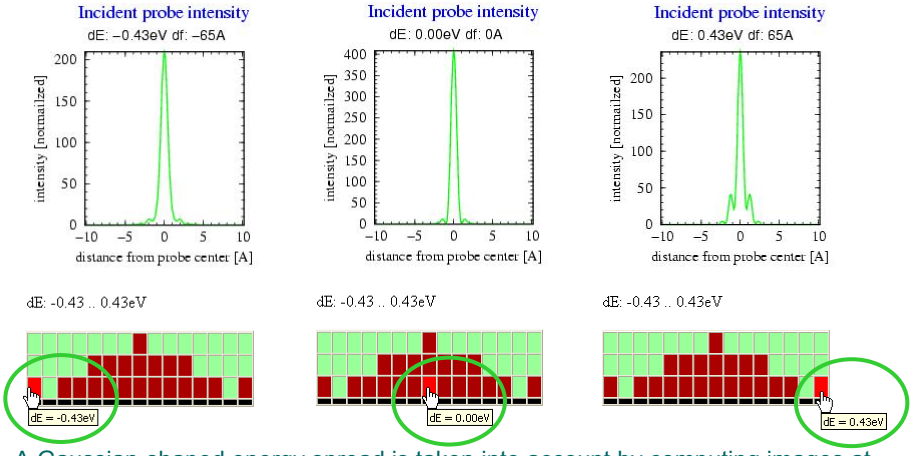


2. Do the (memory consuming) multislice propagation only for one sub-slab at a time.



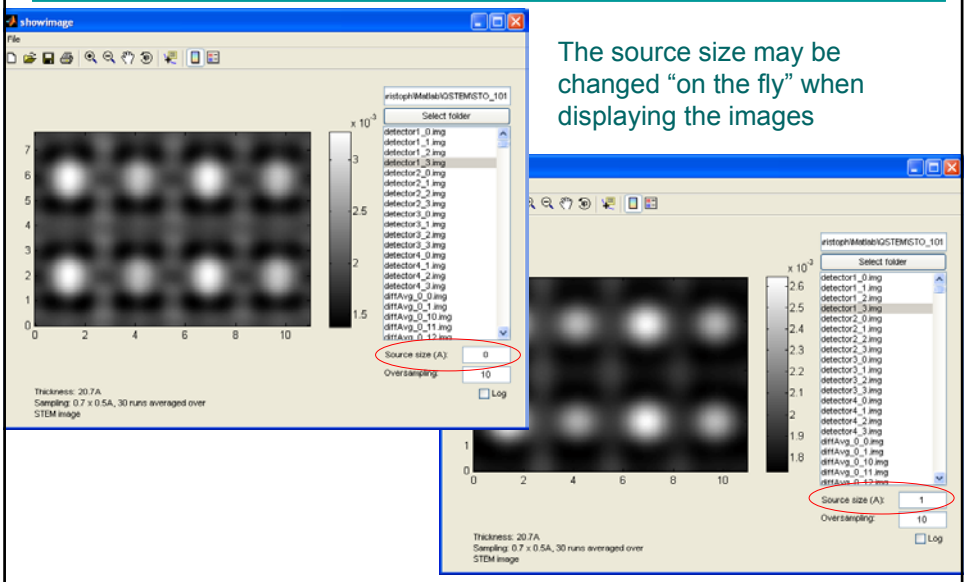
Since intermediate results must be saved to disc, this partitioning takes a bit longer, but there is now no image that cannot be computed

Accounting for energy spread



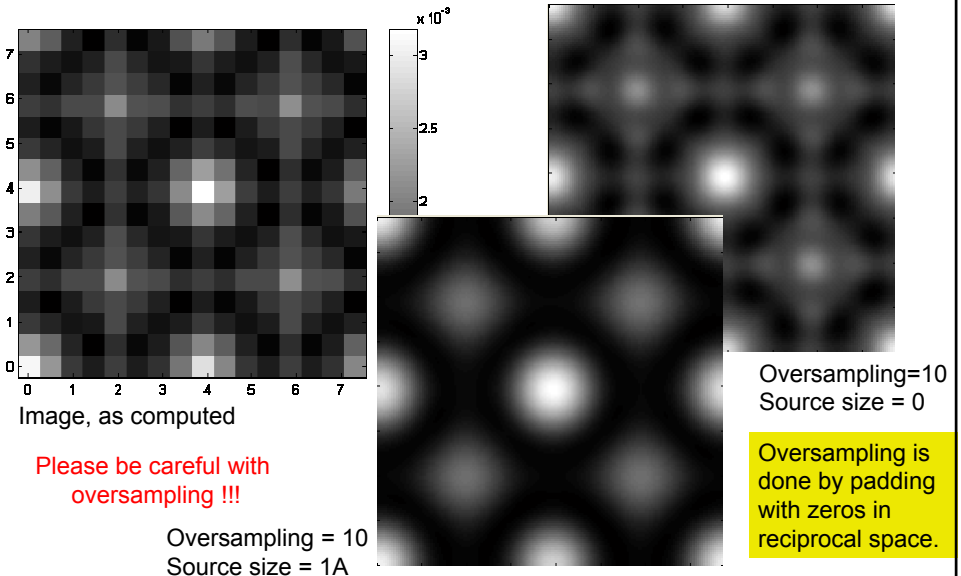
A Gaussian-shaped energy spread is taken into account by computing images at different energies (and with that defocus), as the different probe shapes above demonstrate.

Accounting for source size



The source size may be changed “on the fly” when displaying the images

Interpolation between computed pixels



Image, as computed

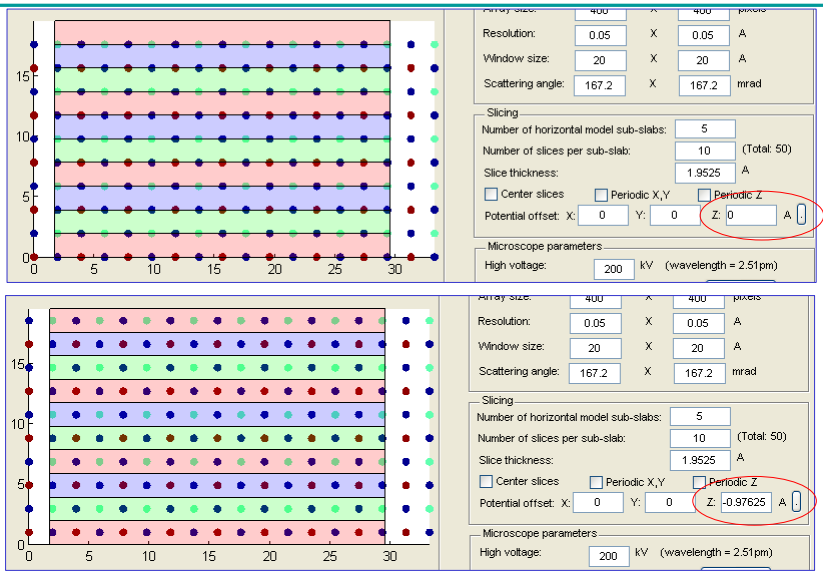
Please be careful with oversampling !!!

Oversampling = 10
Source size = 1A

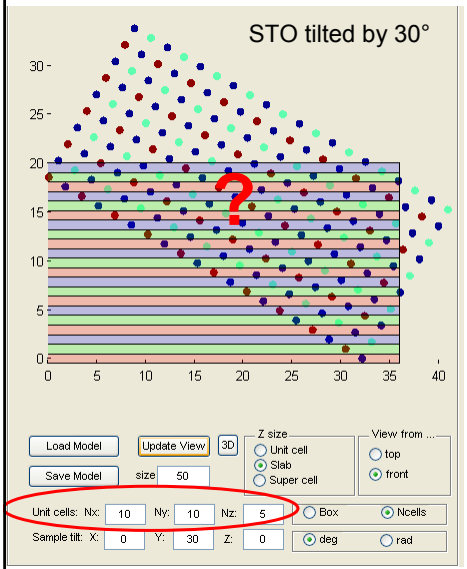
Oversampling=10
Source size = 0

Oversampling is done by padding with zeros in reciprocal space.

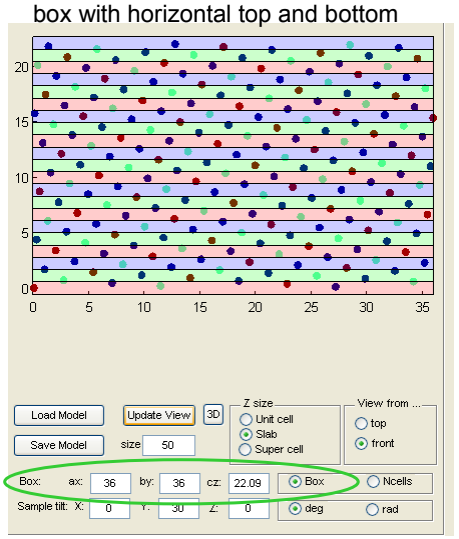
3D slicing of model structure: Potential z-offset



Tilting: Box mode

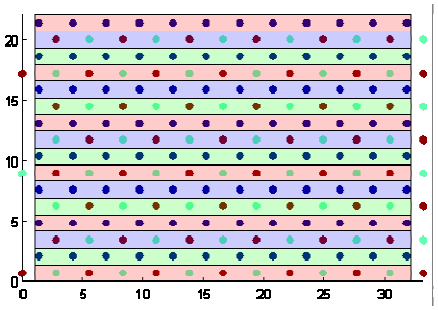


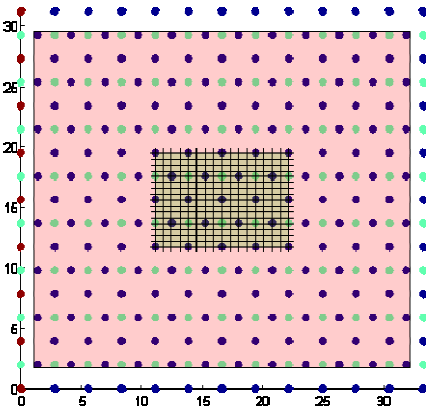
All the atoms are nicely confined in a box with horizontal top and bottom



Different Zone axis? – No problem

$SrTiO_3$ (101)





Box: ax: 34 by: 32 cz: 22.09 Box Ncells

Sample tilt: X: 0 Y: 45 Z: 0 deg rad

Slicing

Number of horizontal model sub-slabs: 1

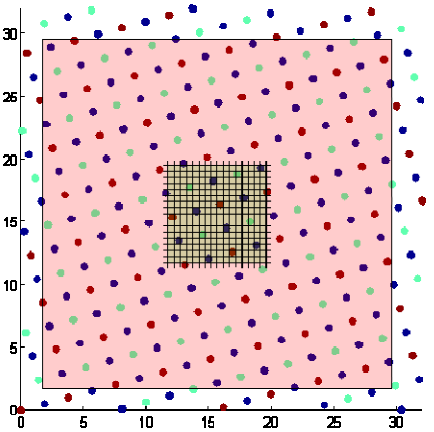
Number of slices per sub-slab: 16 (Total: 16)

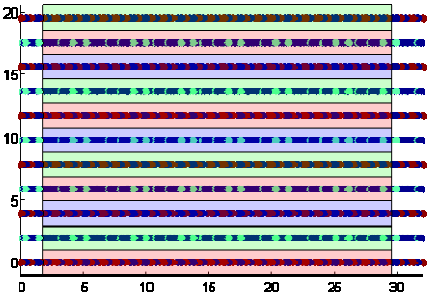
Slice thickness: 1.3806 A

Center slices Periodic X,Y Periodic Z

Potential offset: X: 0 Y: 0 Z: 0.6903 A

Rotating the sample





Box: ax: 32 by: 32 cz: 19.525 Box Ncells

Sample tilt: X: 0 Y: 0 Z: 15 deg rad

Slicing

Number of horizontal model sub-slabs: 1

Number of slices per sub-slab: 10 (Total: 10)

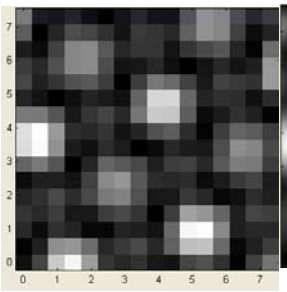
Slice thickness: 1.9525 A

Center slices Periodic X,Y Periodic Z

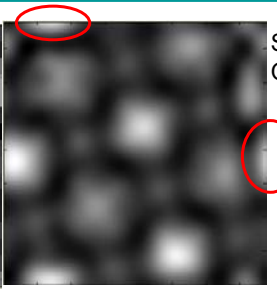
Potential offset: X: 0 Y: 0 Z: 0 A

HAADF STEM images of rotated sample

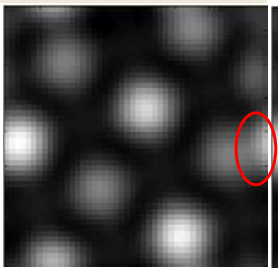
Original image
(no artifacts)



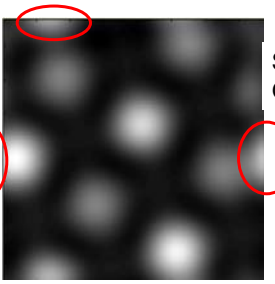
Source size = 0A,
Oversampling = 30



Source size = 1A,
Oversampling = 3



Source size = 1A,
Oversampling = 30



Oversampling artifacts from non-periodic image boundaries