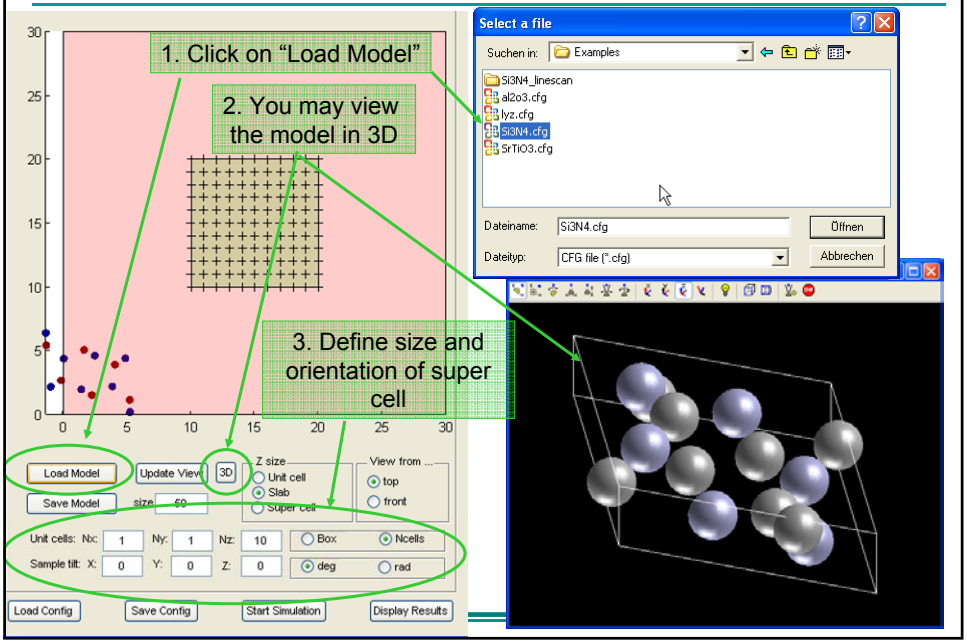
QSTEM Tutorial on
Simulating (HA)ADF/BF-STEM images

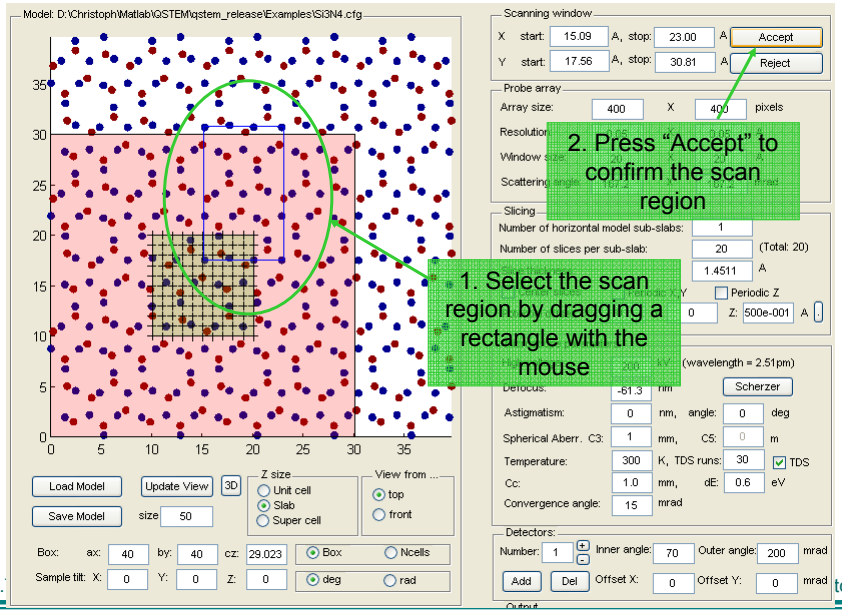
Christoph T. Koch

Stuttgart Center for Electron Microscopy (StEM)
Max-Planck-Institut für Metallforschung, Stuttgart

Step1: Loading the unit cell structure



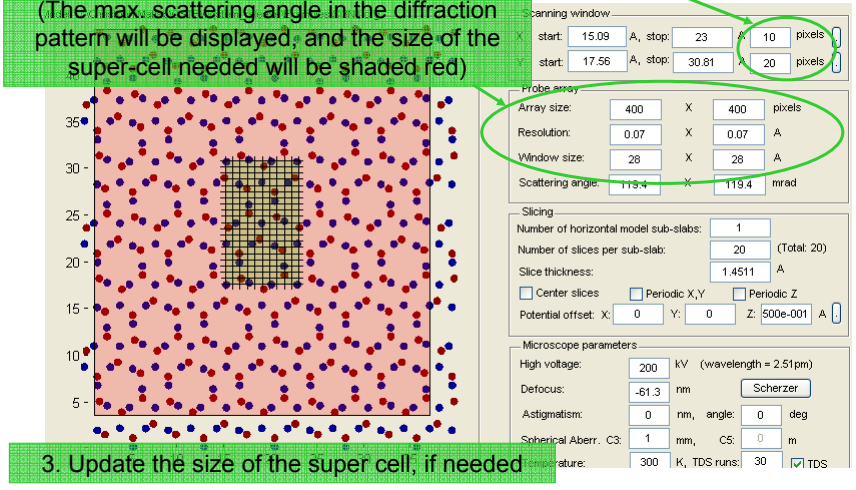
Step2: Define the scan region



Step 3: Setting up the probe array

1. Define number of pixels to be scanned in each direction

2. Define sampling and size of the probe array (The max. scattering angle in the diffraction pattern will be displayed, and the size of the super-cell needed will be shaded red)



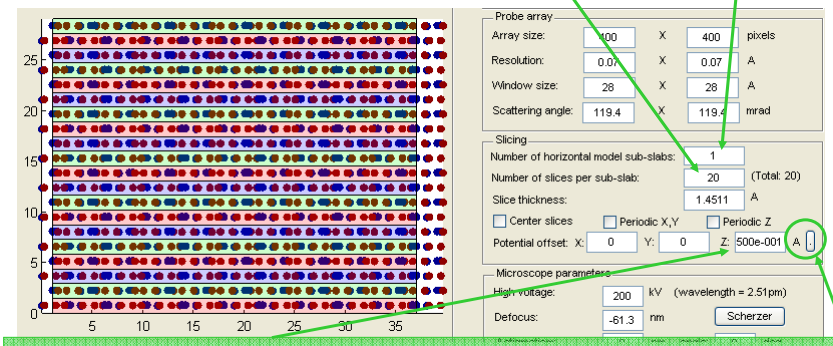
3. Update the size of the super cell, if needed

Step 4: Define the slicing

1. Switch to “View from … front”

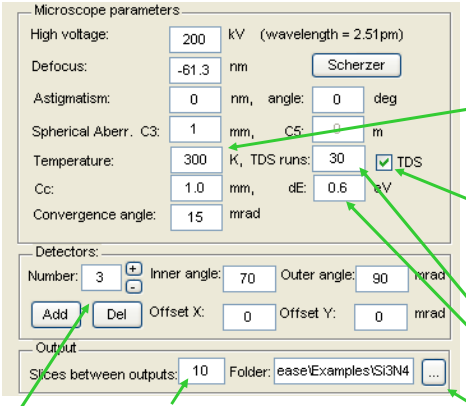
2. Set “Number of .. sub-slabs” according to the amount of RAM available in your machine

3. Set “... Slices per sub-slab” so that there is 1 atomic layer per slice (press “Update View” to verify)



4. Set Potential offset Z” to position atom layers in the center of the slices. Pressing the button to the right will set it to ½ the slice thickness.

Step 5: Setting up microscopy parameters



The temperature allows an overall scaling of the Debye-Waller factors provided with the unit cell atom positions:

$$DW_{eff} = DW \cdot \sqrt{Temperature / 300}$$

Should be turned on for quantitative STEM simulations. Will otherwise result in simple Debye-Waller attenuation of Bragg beams but TDS will be missing.

Number of calculations to average over. (can be smaller for thick samples)

Energy spread of source.

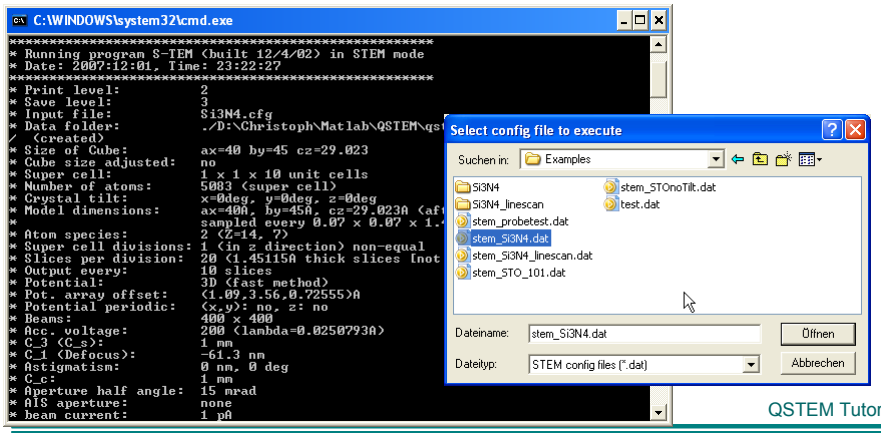
Compute intermediate images every N slices

Add, delete, and modify detectors (default: 1: 70 .. 200 mrad, 2: 0 .. 40 mrad). Detectors can also be shifted in the diffraction plane.

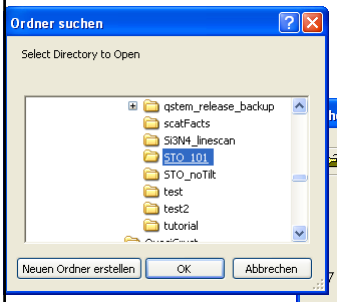
Define a folder for saving images, wave functions, and diffraction patterns.

Step 6: Save and run

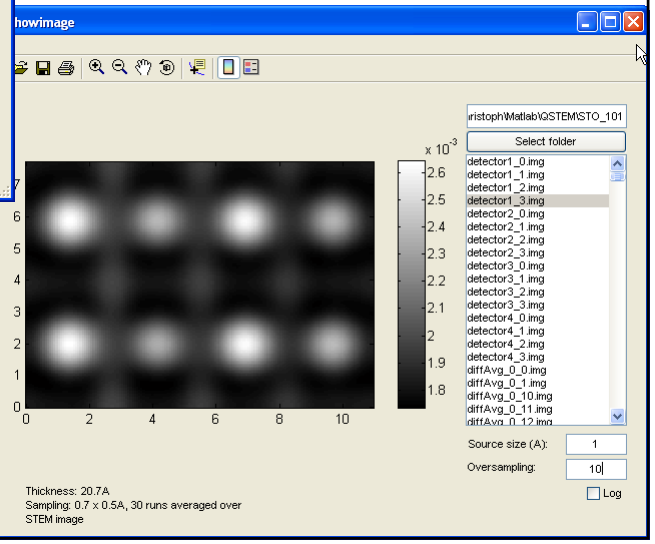
1. Save the configuration to a file using “Save Config”
2. Run the just saved (or any other) configuration using “Start Simulation”
   (Note: many different configurations may be run simultaneously [makes sense on a multiprocessor machine], but they all should have different output folders, otherwise, their results will be overwritten)



Step 7: View the results



1. Press “Display Results”, and wait for a new window named “showimage” to open

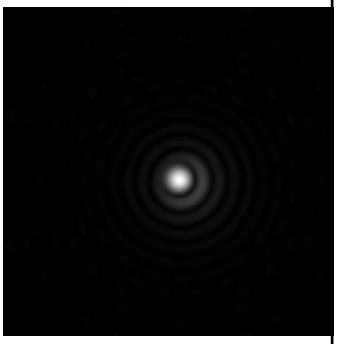


2. Select the image / diffraction pattern / wave function and set a suitable oversampling and source size.
(Note: Complex wave functions may be displayed in different ways.)

C.T. Koch

Exercise 1: Effect of probe astigmatism

1. Load the configuration file “stem_probetest.dat” This sets up a single slice without any potential in it (it is still necessary to have a super-cell as large as the scan window though). It also turns off TDS, since we only want to look at the wave function anyway.
2. Change the astigmatism magnitude and angle to different settings. Also play with Cs and defocus.
3. Save the configuration file.
4. Run the simulation and display the wave function.



Exercise 2: Evolution of wave function

1. Load the configuration file stem_STO_4x4.dat. Make sure that the number of pixels in the scan is not set too high (4 x 4 should be enough for this test.
2. Start the simulation
3. Open the “Task Manager” to see how much memory is being allocated by the simulation (look for “stem3.exe”)
4. Look at the wave function by pressing “Display Results”
5. Double the number of unit cells in z-direction, change the output folder save and run again.
6. See how much further the wave function has spread (look at both, the modulus and the intensity).
7. Compare the STEM images and their thickness evolution computed with TDS = ‘off’ with those that have been simulated with TDS = ‘on’ (5 averages suffices). Use Oversampling =10 to display the STEM images.