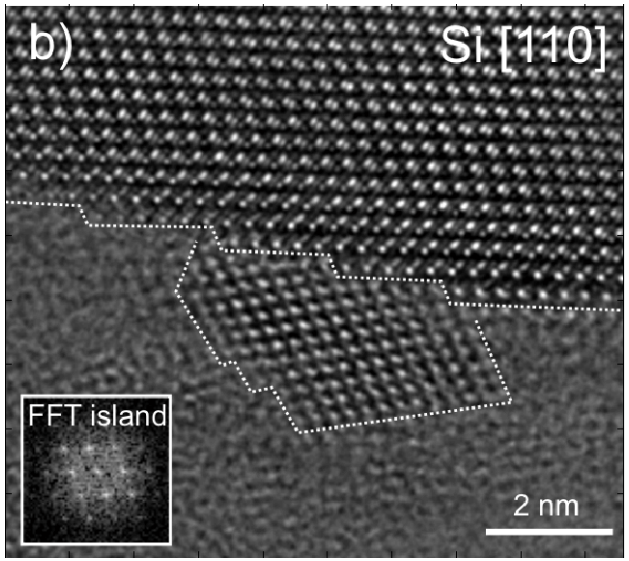
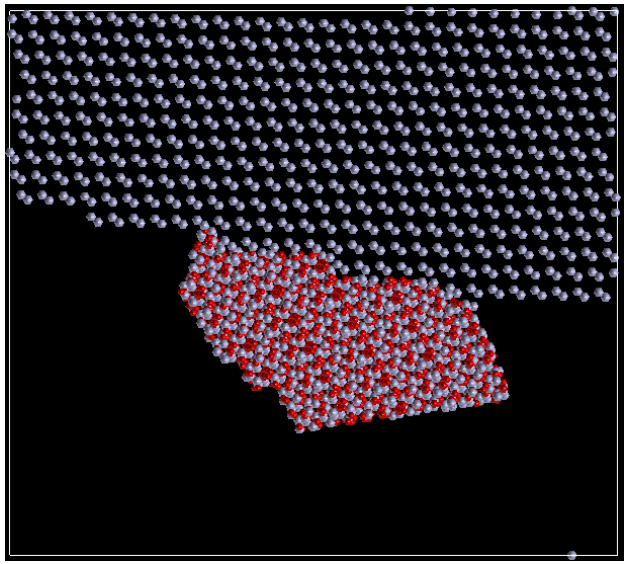
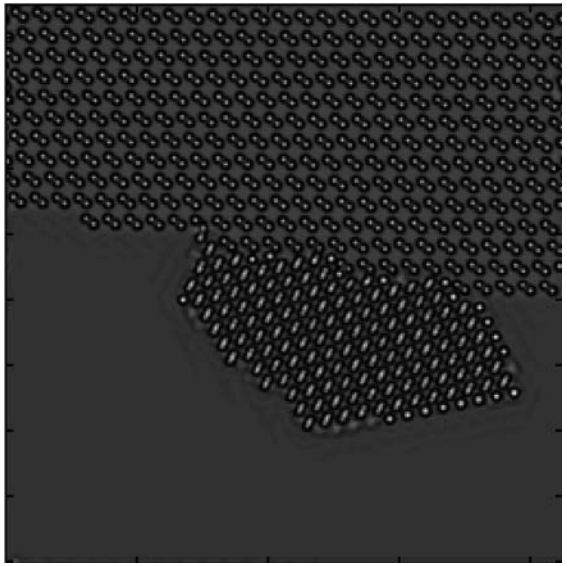
qmb: QSTEM Model Builder







Christoph T. Koch

Stuttgart Center for Electron Microscopy

Max Planck Institute for Intelligent Systems

Heisenbergstr. 3, 70569 Stuttgart

About the qmb Software

Motivation:
If you have a TEM image of an interface, a surface, or a nanoparticle, you might be interested in the atomic structure of the object you are observing.

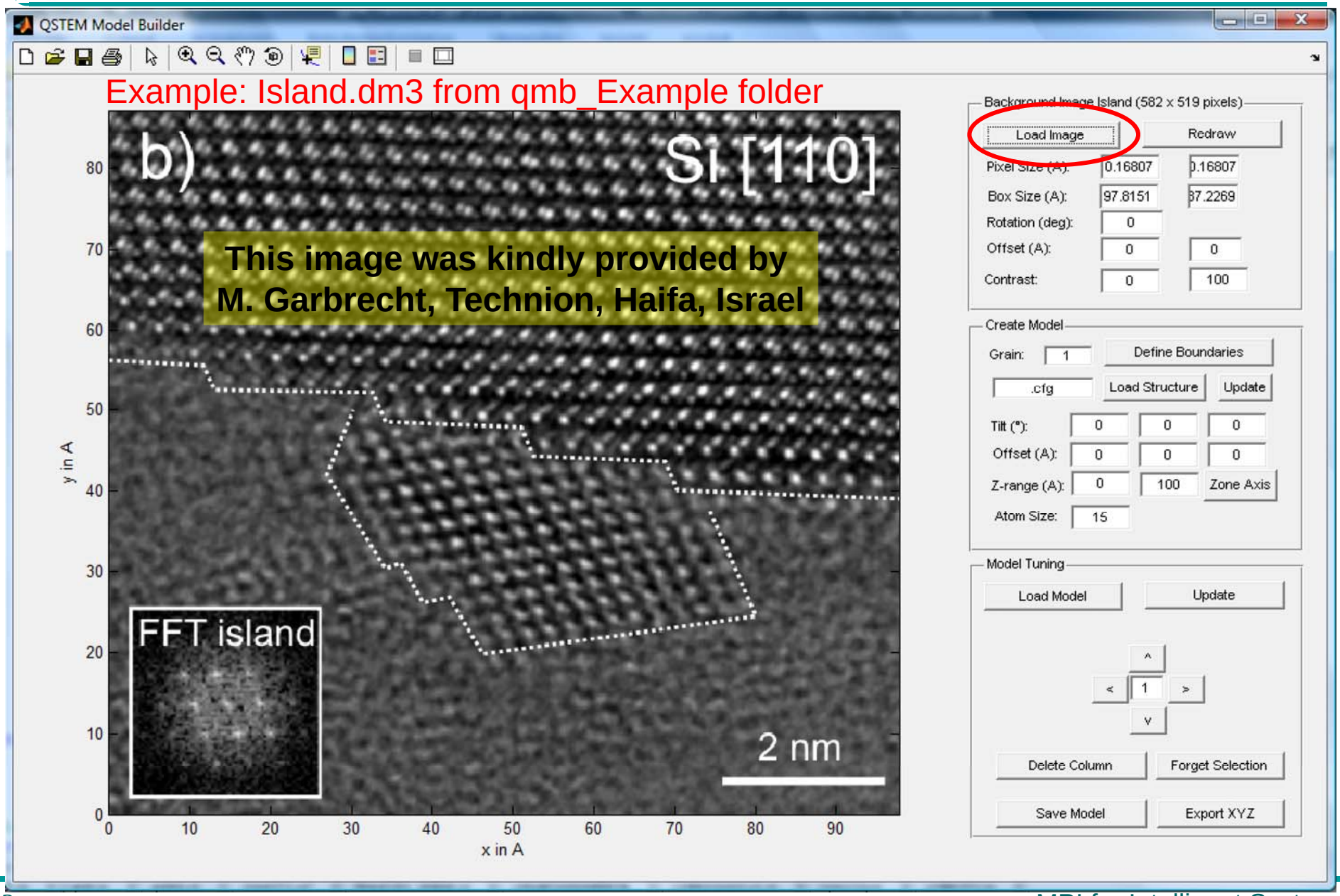
This software may help you to generate an atomic model by superimposing whatever you create on top of the image you already have.

Implementation:
This code is intended to be easy to use, but certainly does not fulfill all of your dreams of what the ideal software for such a purpose should be able to do.

For images, qmb can read .img, .dm3, .tif, .jpg, and a few more common image formats. In the case of .dm3 and .img qmb will also automatically ready the pixel size in A.

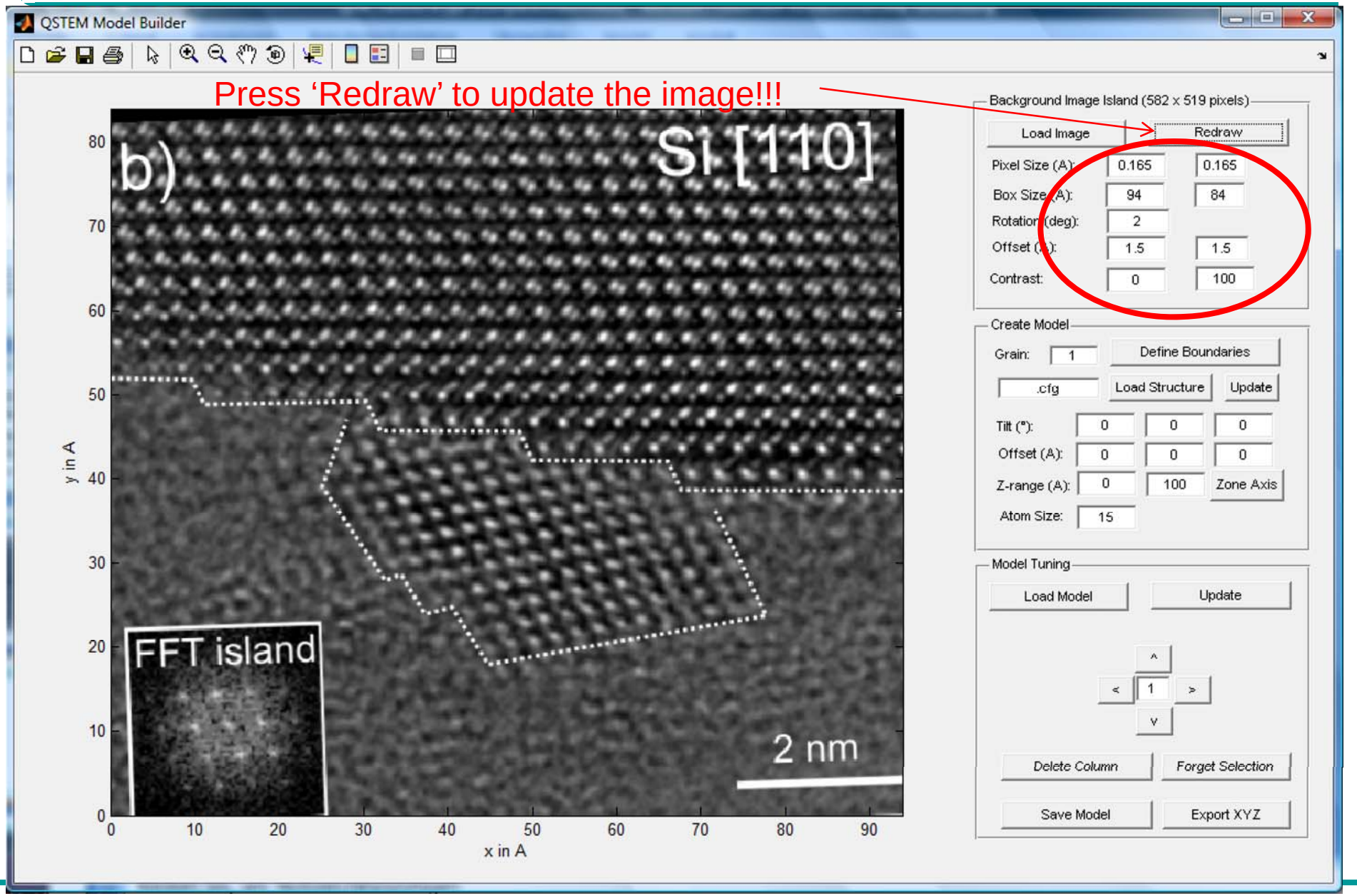
For atomic structures qmb reads .cfg format and can write .cfg as well as .xyz files.

Step 1: Load a HRTEM image



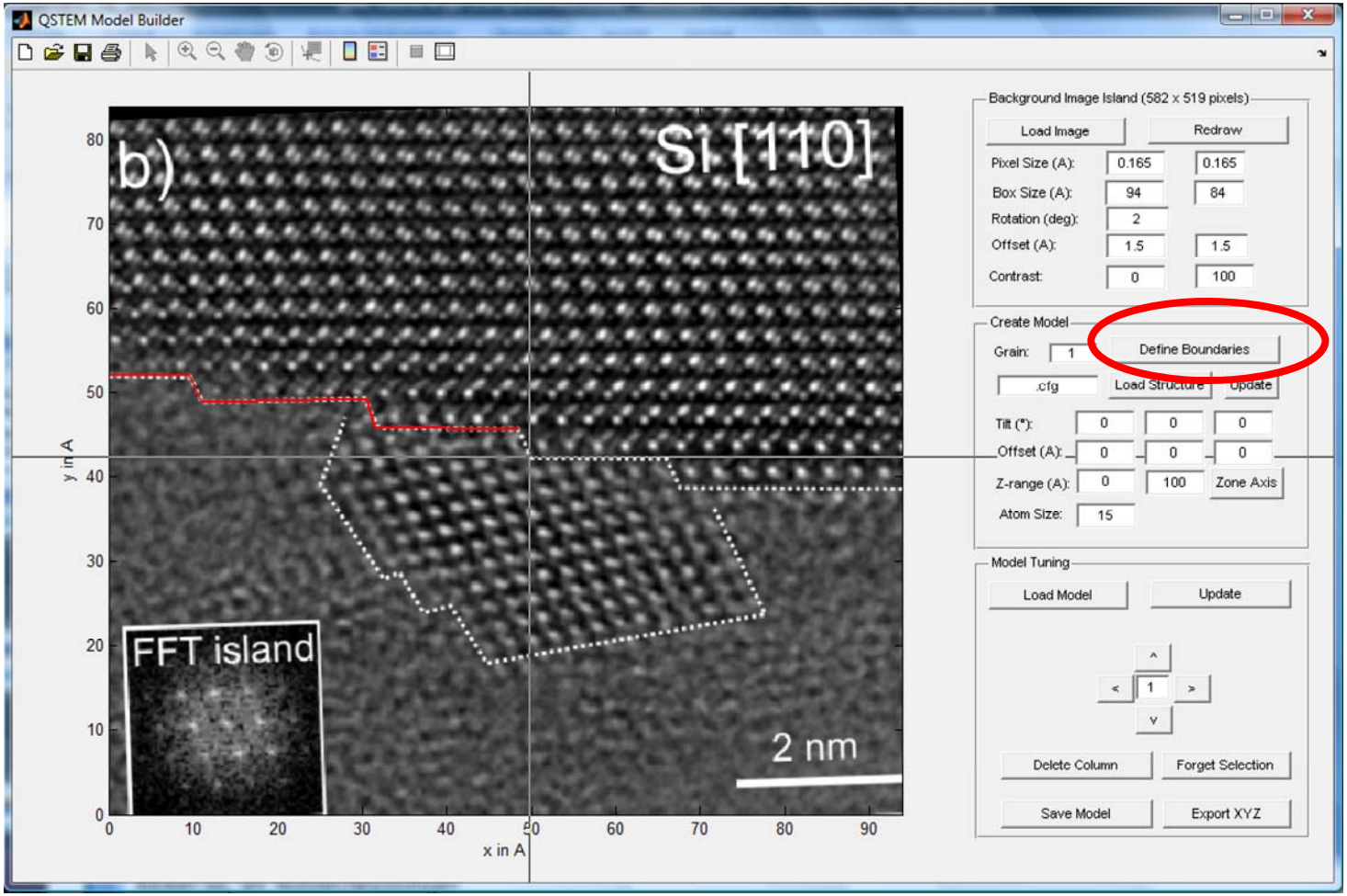
Step 2: Adjust image (rotation, offset, scale…)

STEM Stuttgart Center for Electron Microscopy



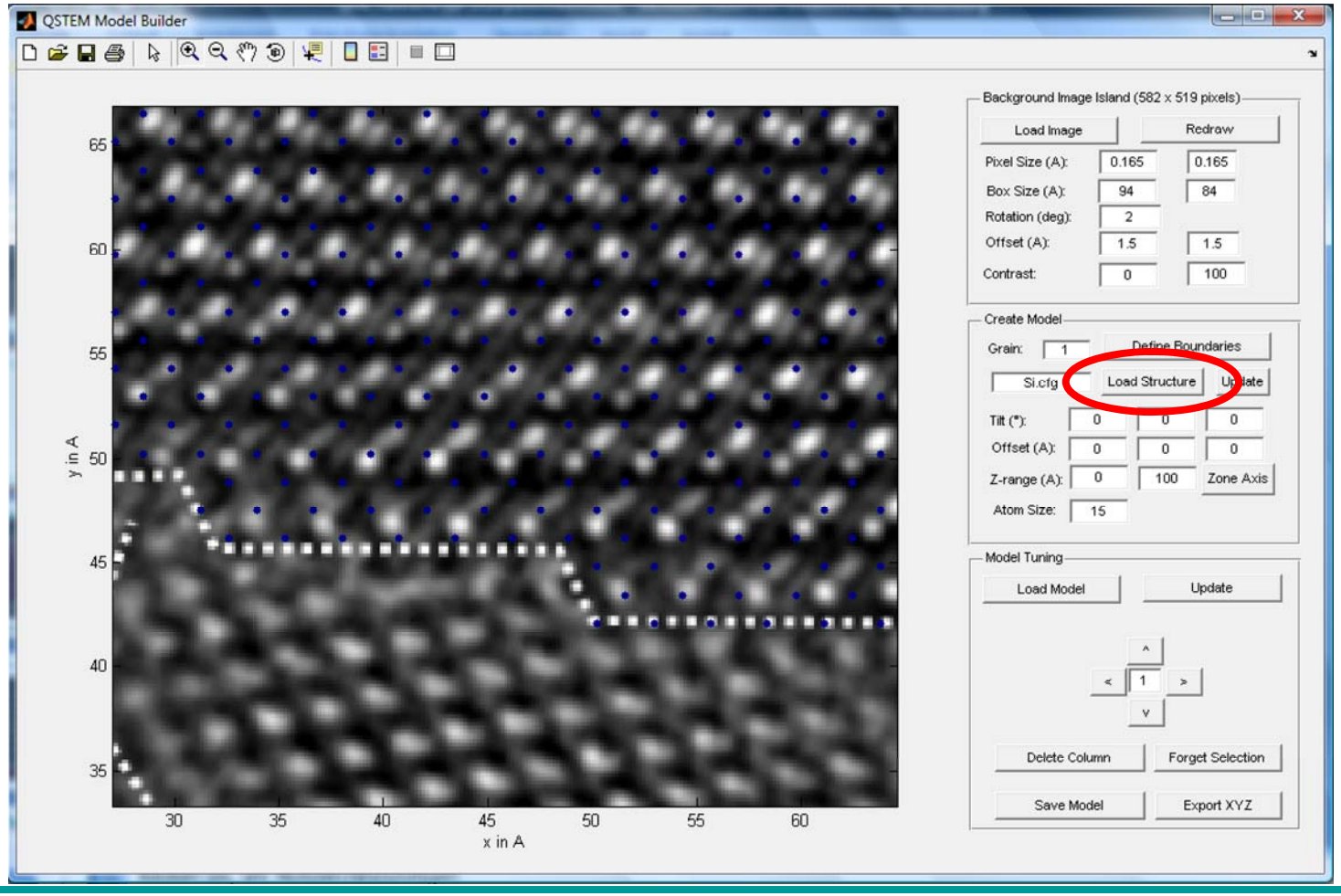
Step 3: Outline the area covered by Grain 1

1. Press ‘Define Boundaries’
2. Use left mouse button to define vertices of polygonal outline of the grain
3. Close polygon by clicking the right mouse button (this will connect the start and end points of the outline)



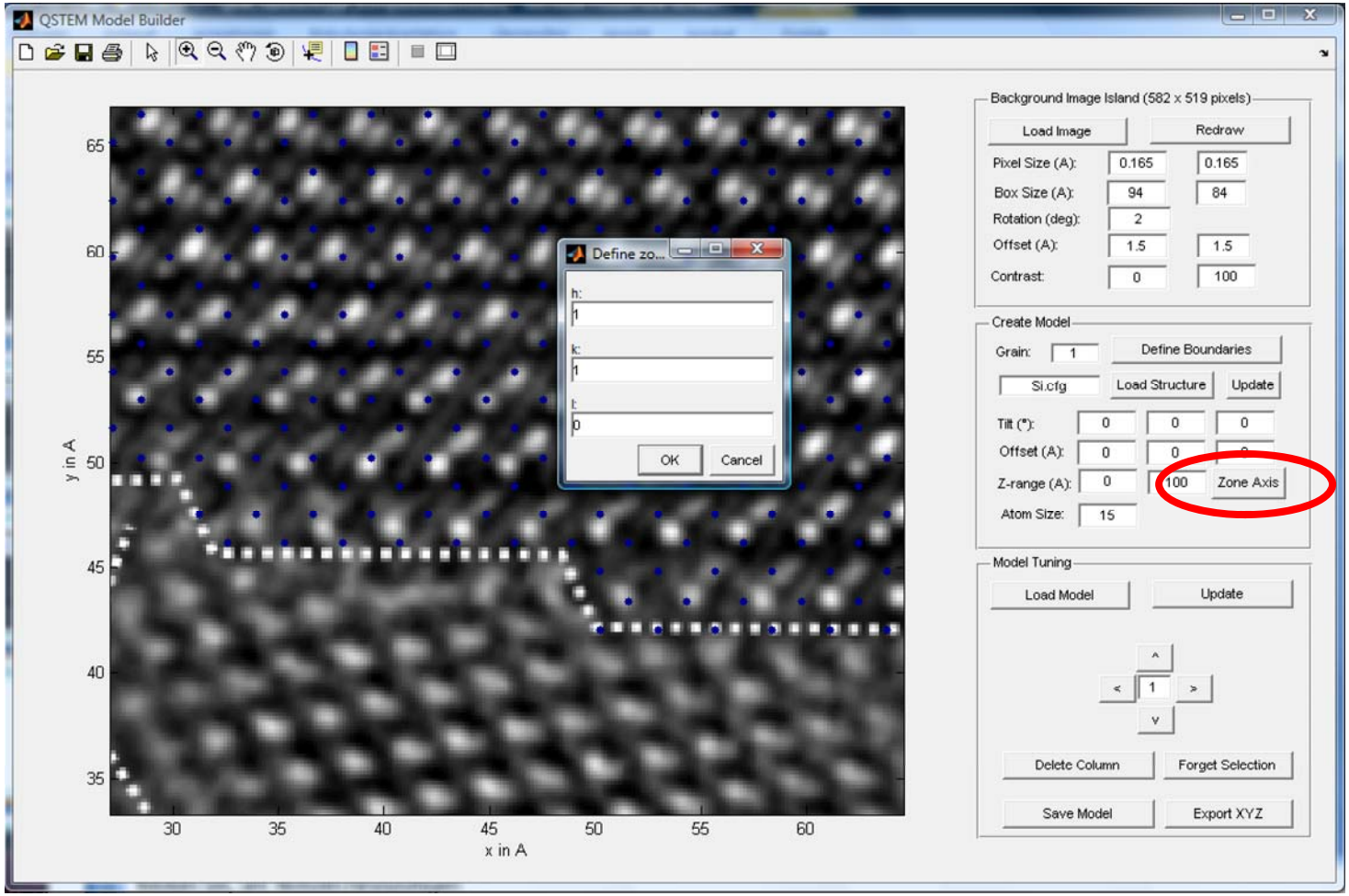
Step 4: Load .cfg file of Grain 1's structure

1. Press 'Load Structure' and select the .cfg file you want to fill this grain with (e.g. use Si.cfg from the qmb_Example folder)
2. You may use the toolbar buttons to zoom in/out and pan



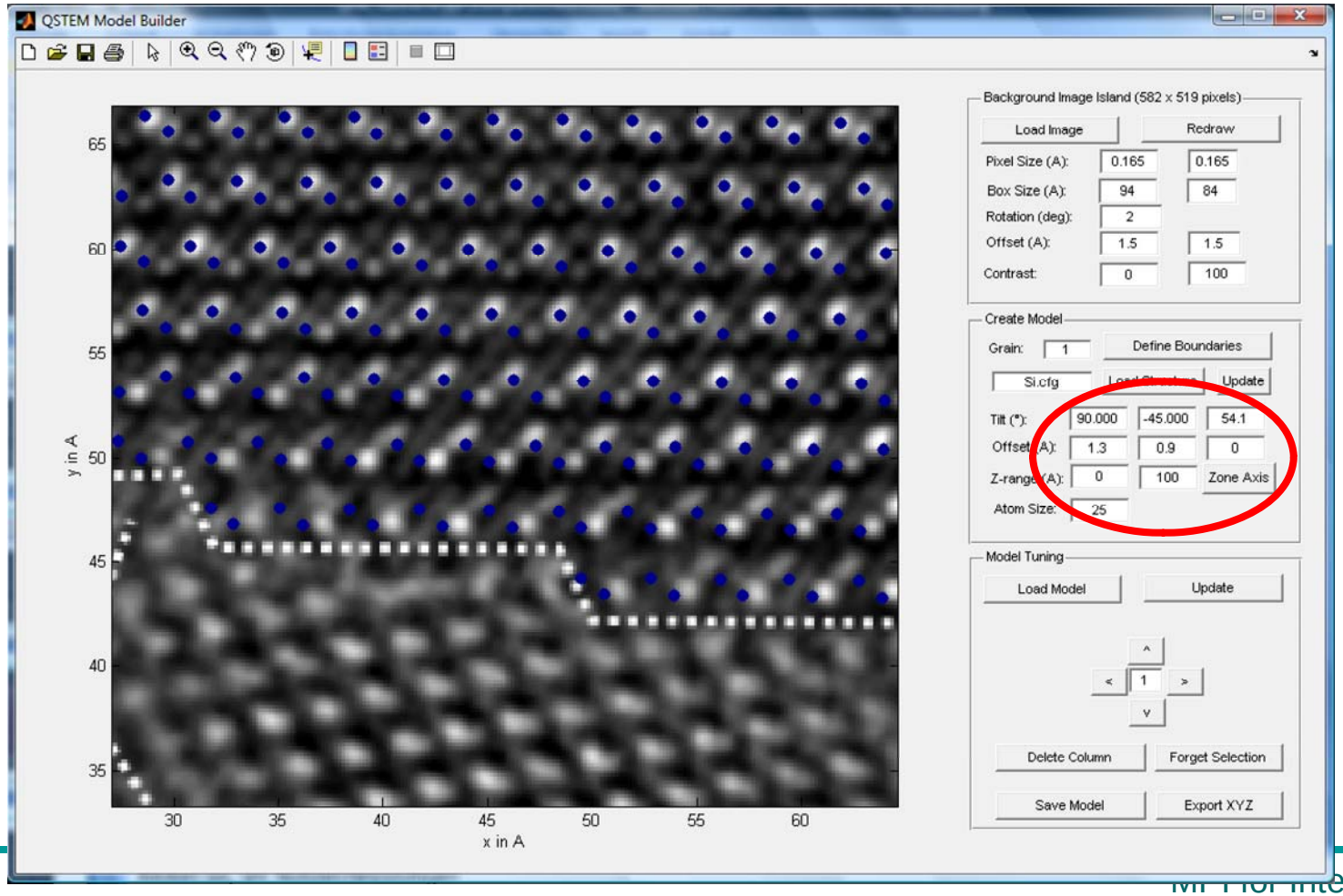
Step 5: Define the zone axis

1. Press ‘Zone Axis’
2. Define h,k, and l of your desired zone axis (this defines the required tilt angles)
   You may also change these angles to deviate from exact zone axis
3. Press ‘Update’ in the ‘Create Model’ box to display the rotated structure of this grain.



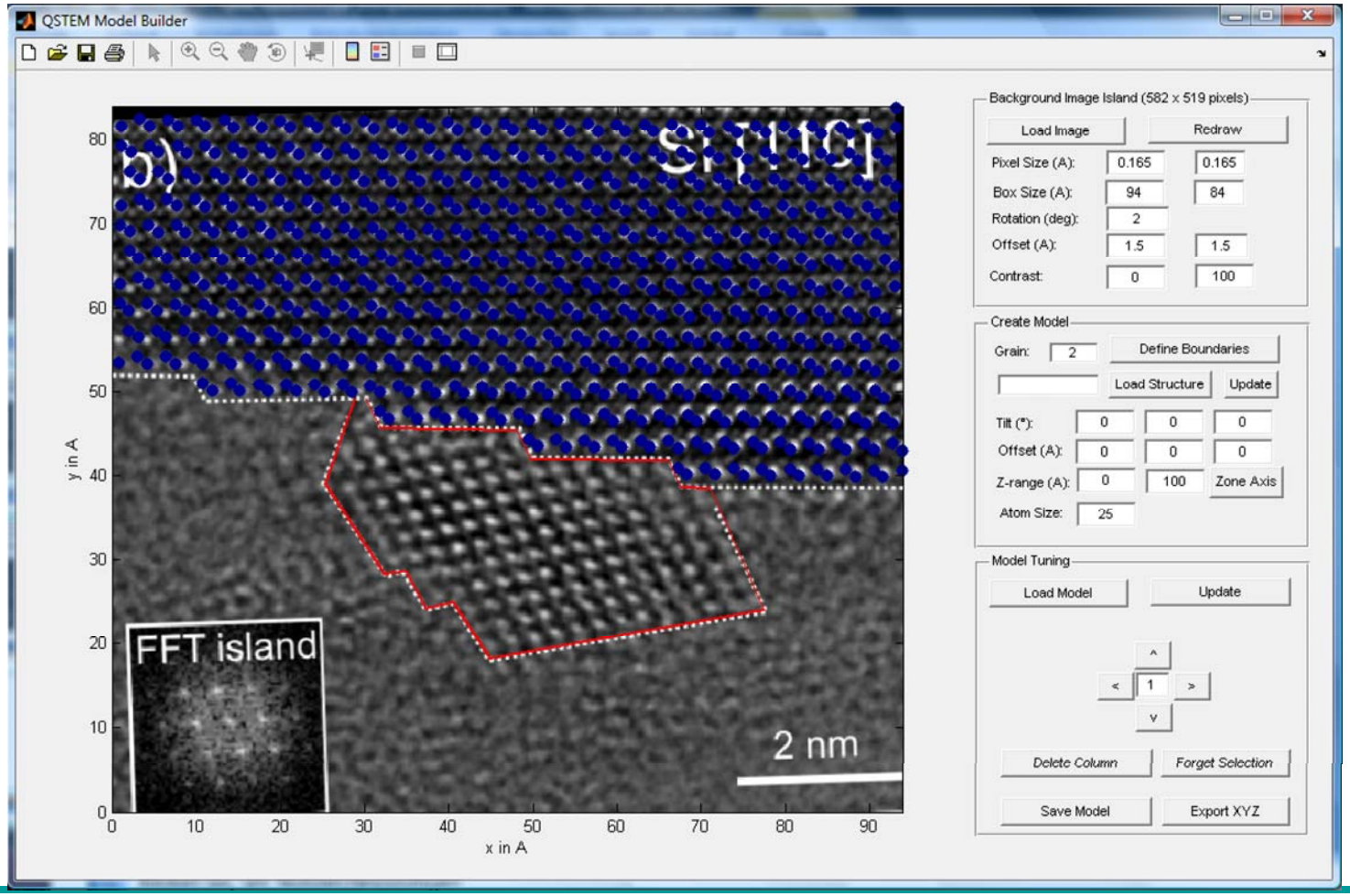
Step 6: Define z-rotation and offsets

1. The first 2 tilt parameters define the zone axis, and the 3rd the rotation of this zone
2. Use x- and y- offsets to shift atomic columns on top of the image features you think they correspond to (ideal are: NCSI contrast or phase of exit wave)
3. Define the z-range of the current grain (here from thickness 0 .. 10 nm)
4. Atom Size changes size of atom-representing dots (zoom-independent).



Step 6: Add next grain

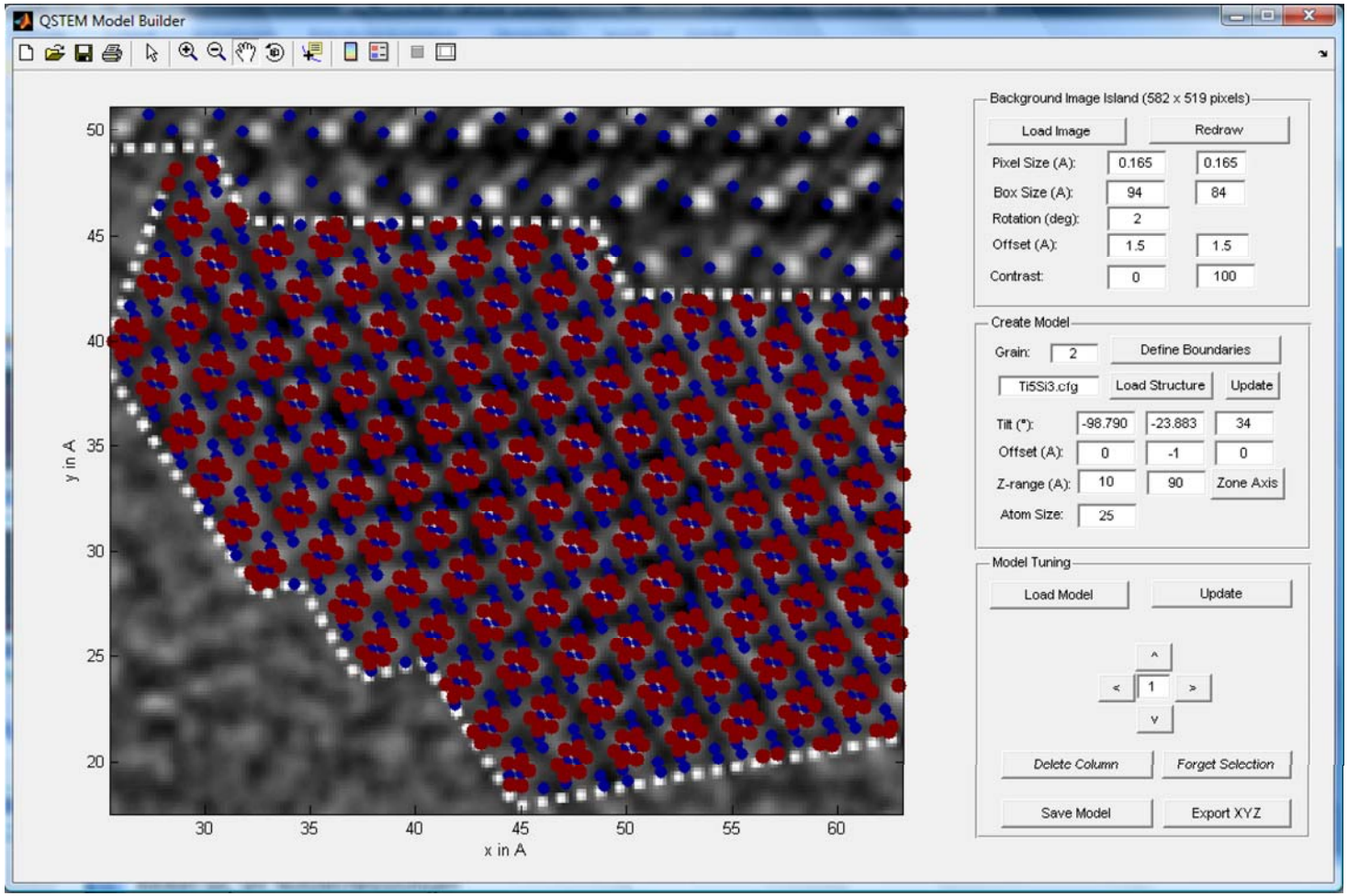
1. Change the grain index to ‘2’
2. Press ‘Define Boundaries’ and outline the next grain



Step 7: Align atomic columns with image

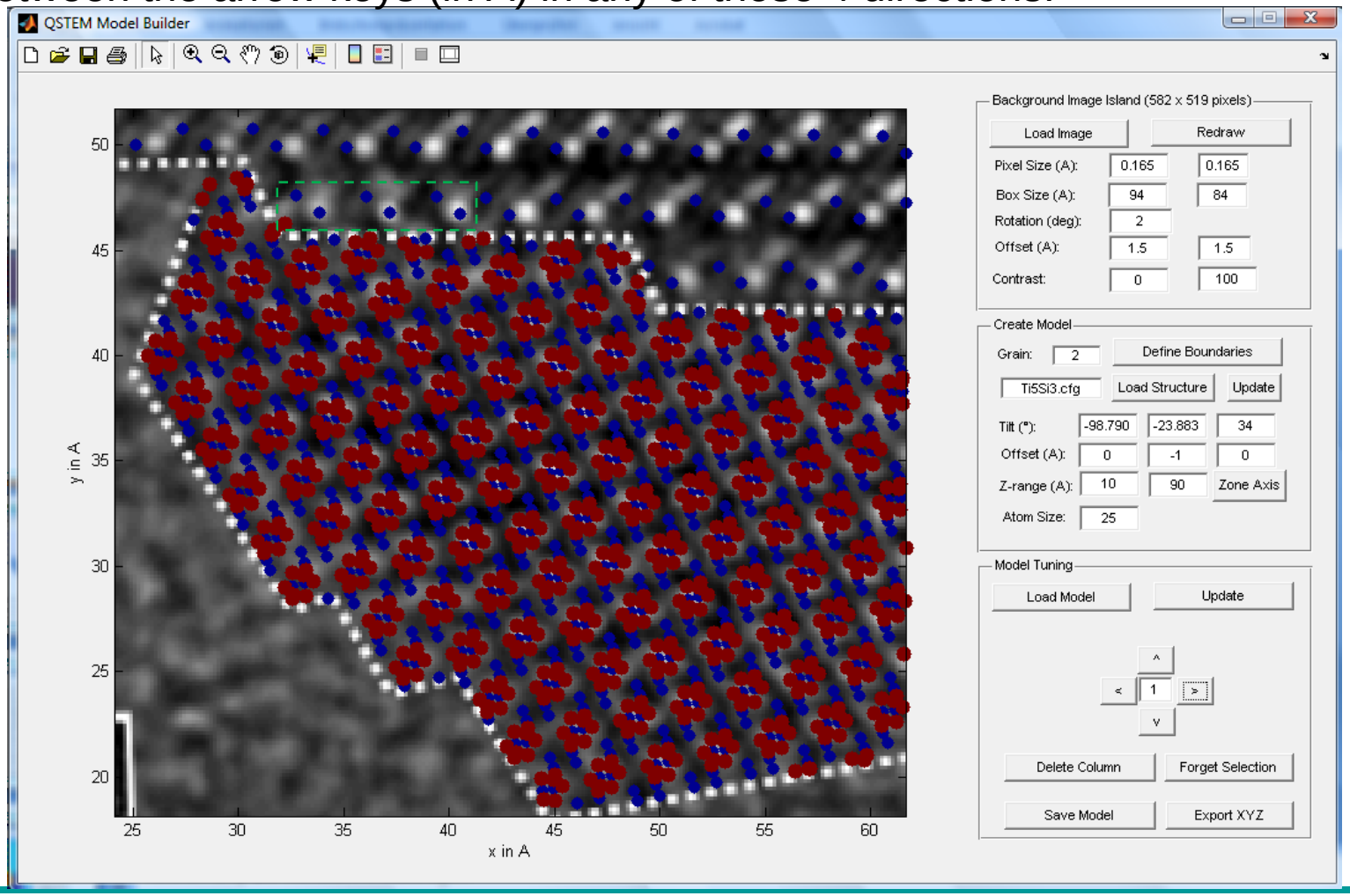
Repeat steps 4 through 6 for grain 2

- Note: the size of the atom-representing dots is independent of the zoom on the image
- If all the grains are defined, press ‘Update’ in the ‘Model Tuning’ box.



Step 8: Fine-Tuning the Model

1. Draw a box around the atomic columns you want to modify
   (if the rubberbox does not appear, press ‘Update’ in the ‘Model Tuning’ box)
2. You can now either delete these columns or shift them by the amount defined between the arrow keys (in Å) in any of those 4 directions.



Step 9: Save the finished model

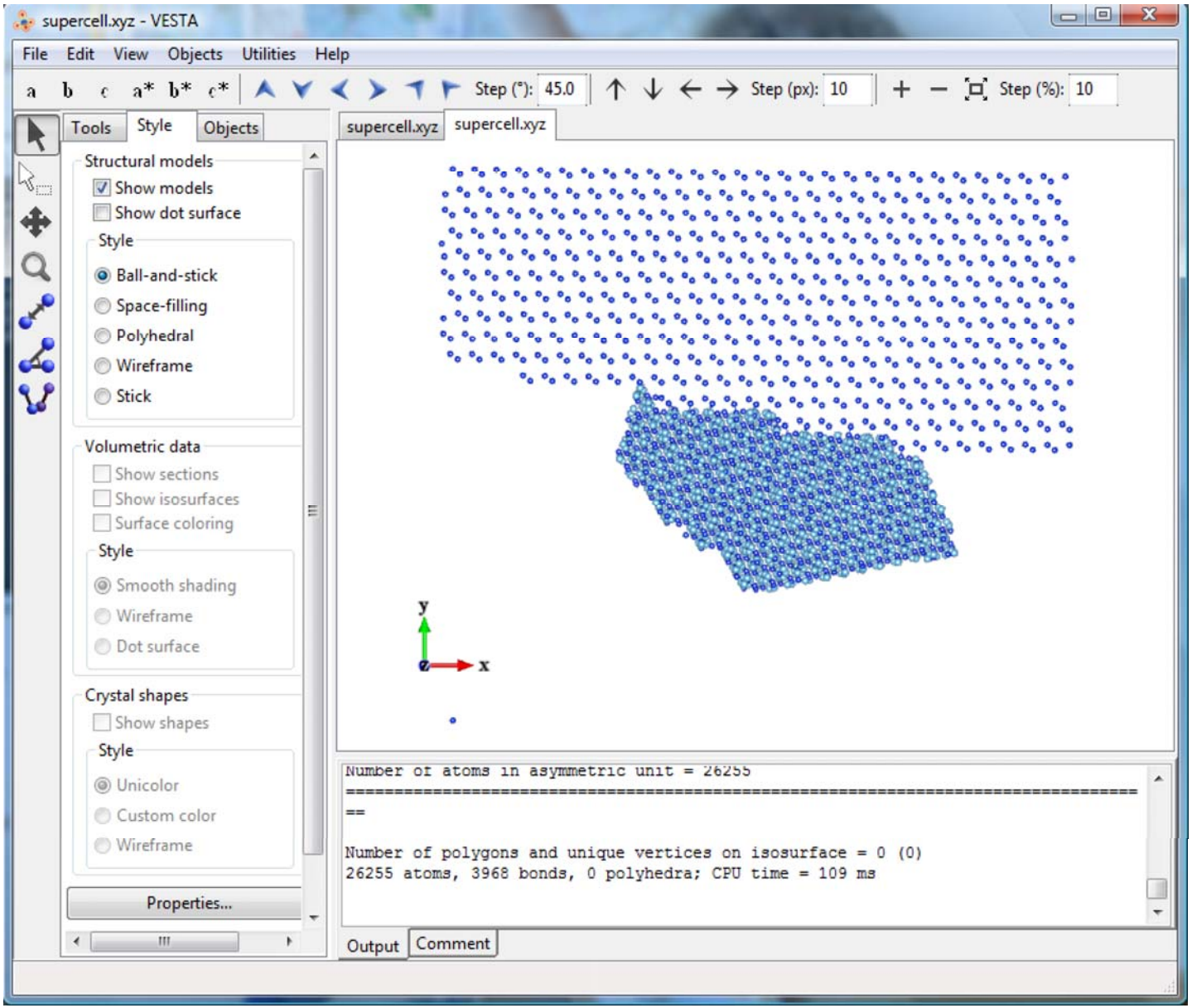
Finally, you can save the model in either .cfg format (for continued cutting in 3D space using gbmaker or for continuing with (qstem) TEM image simulations)

or

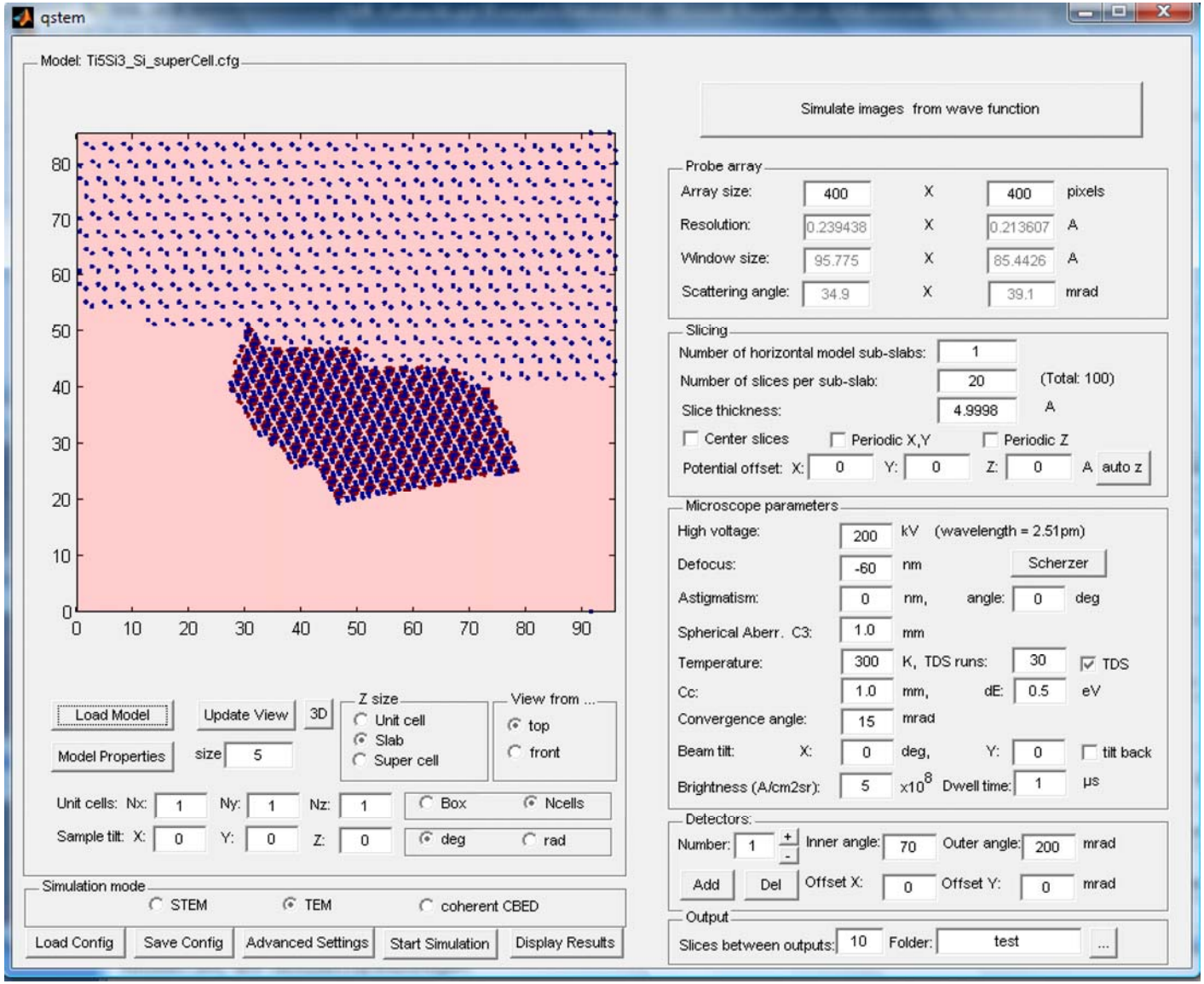
You can export the atomic structure in .xyz format (for display and further processing in other tools*)

* e.g. Vesta (http://www.geocities.jp/kmo_mma/crystal/en/vesta.html)

XYZ Model loaded into Vesta

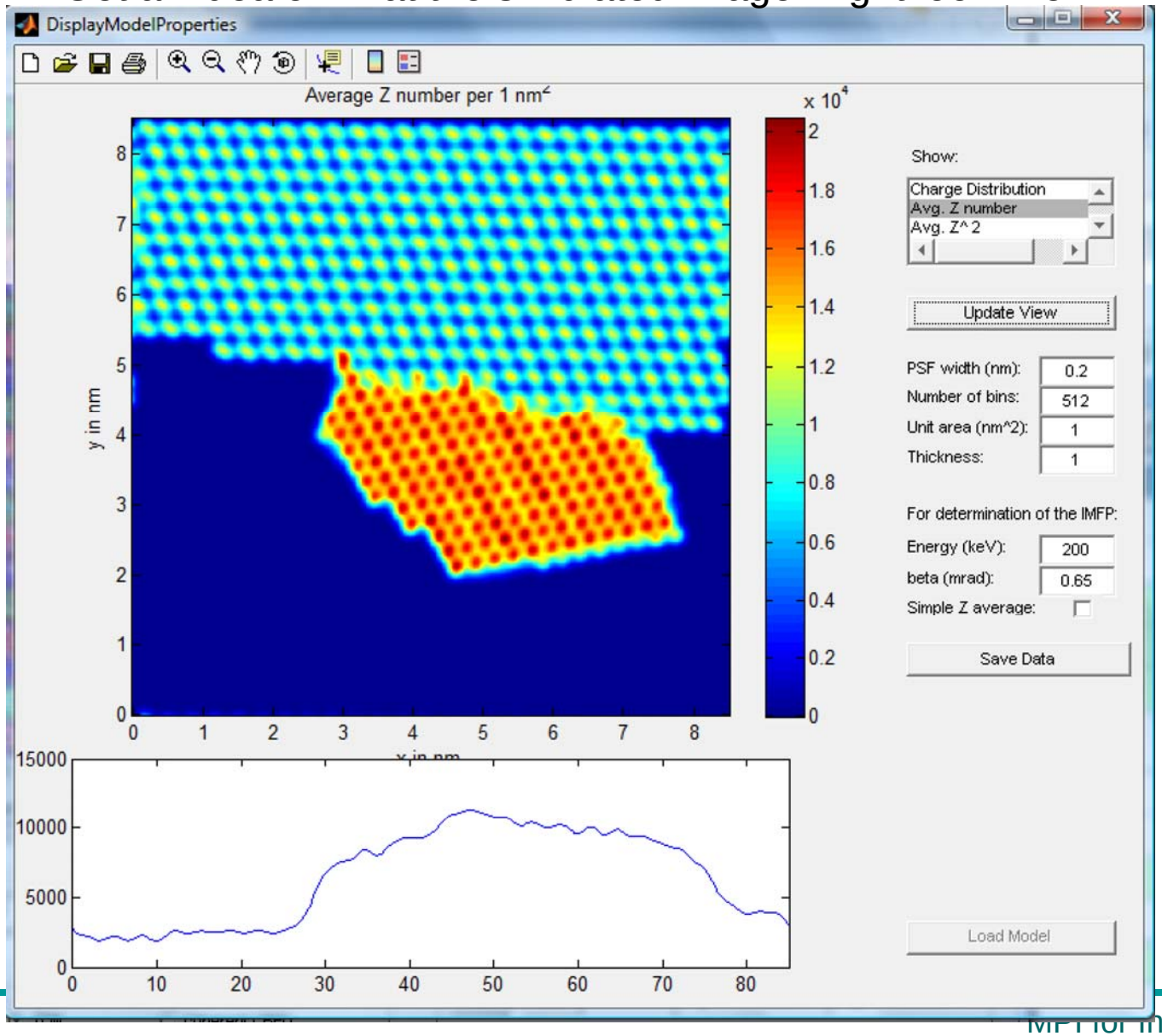


Model loaded into qstem



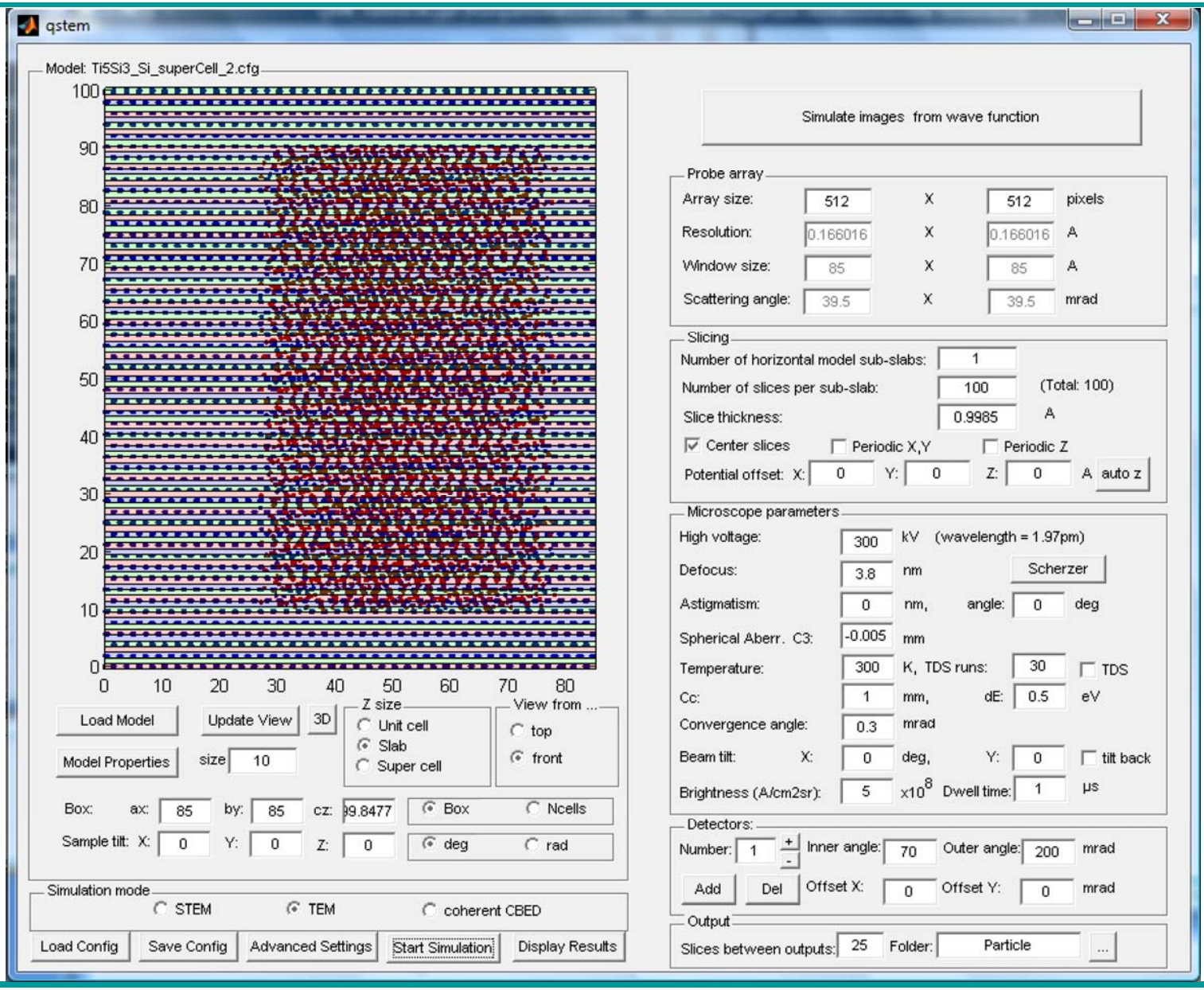
qstem 'Model Properties'

Get an idea of what the simulated image might look like …



Front view: 10 nm thick Si + 8 nm thick particle

STEM Stuttgart Center for Electron Microscopy



Simulate Images