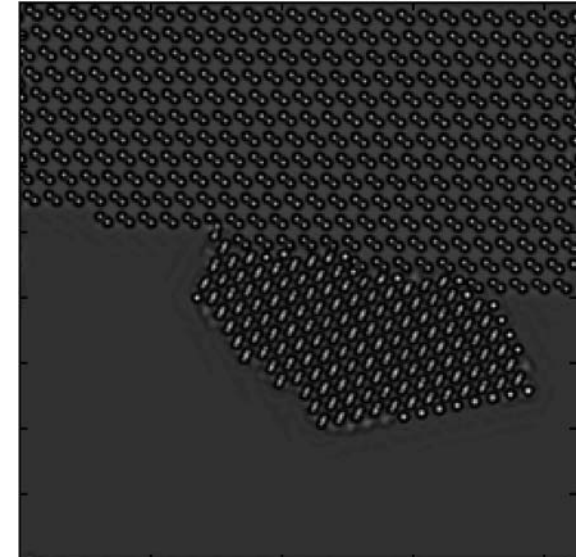
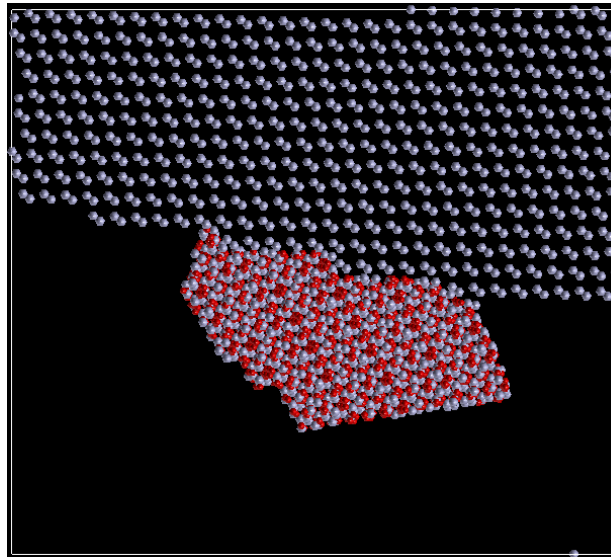
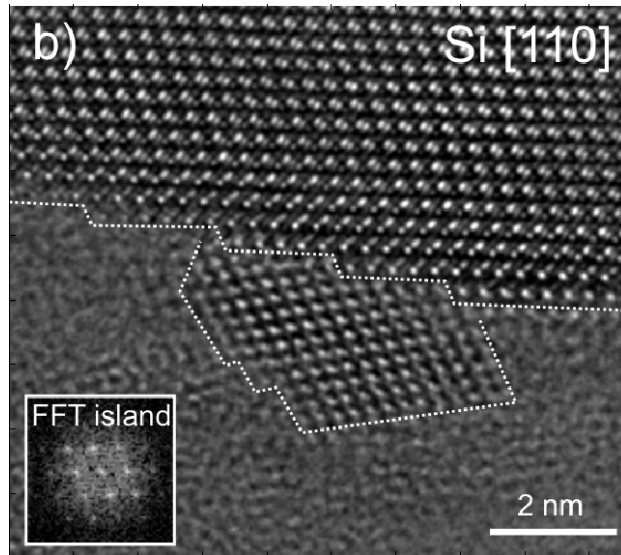


qmb: QSTEM Model Builder



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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 read the pixel size in Å.

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



QSTEM Model Builder

Example: Island.dm3 from qmb_Example folder

b) Si [110]

This image was kindly provided by M. Garbrecht, Technion, Haifa, Israel

FFT island

2 nm

Background Image Island (582 x 519 pixels)

Load Image Redraw

Pixel Size (Å): 0.16807 0.16807

Box Size (Å): 97.8151 87.2269

Rotation (deg): 0

Offset (Å): 0 0

Contrast: 0 100

Create Model

Grain: 1 Define Boundaries

.cfg Load Structure Update

Tilt (°): 0 0 0

Offset (Å): 0 0 0

Z-range (Å): 0 100 Zone Axis

Atom Size: 15

Model Tuning

Load Model Update

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v

Delete Column Forget Selection

Save Model Export XYZ

x in Å

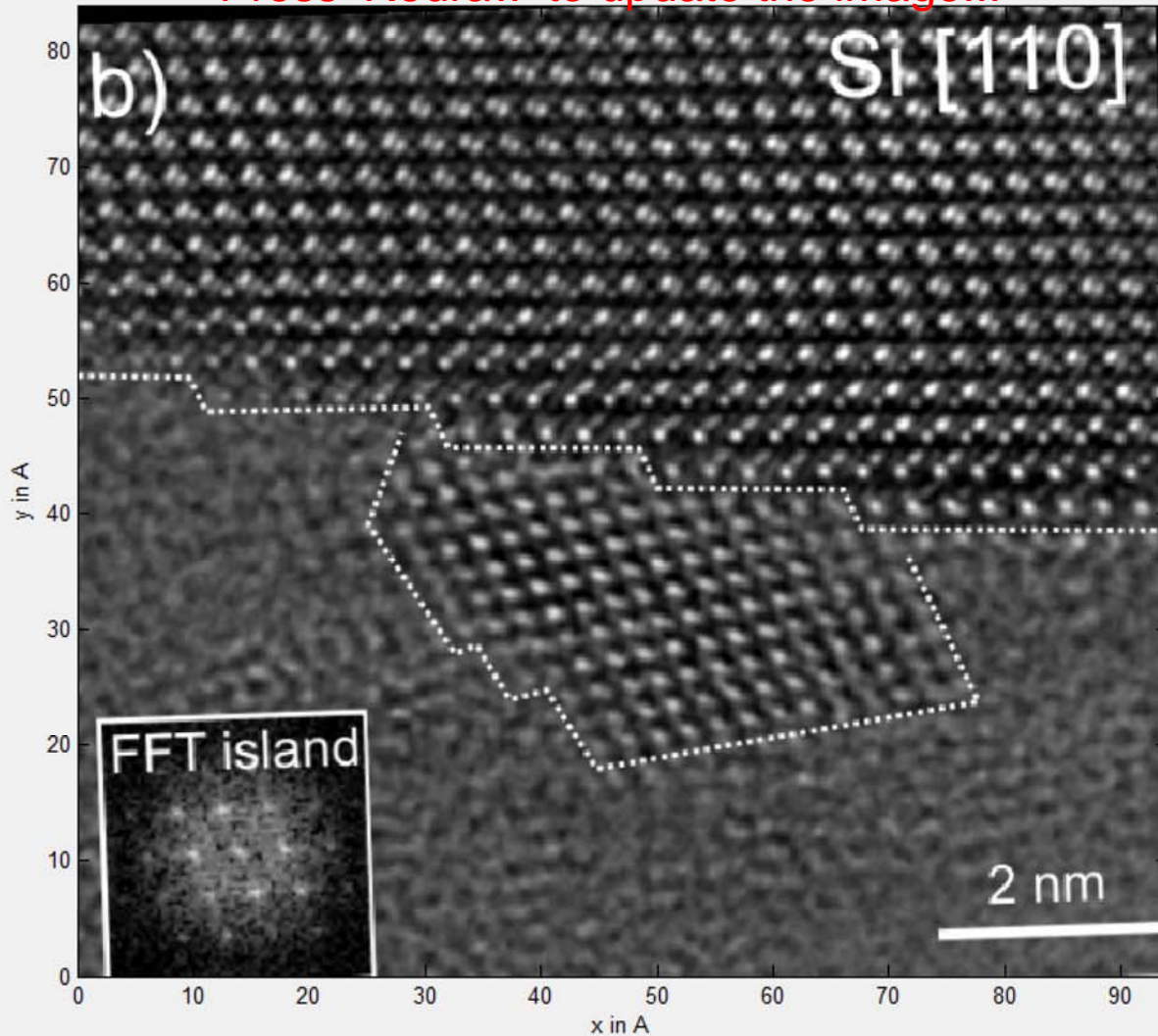
y in Å

STEM Step 2: Adjust image (rotation, offset, scale...)

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Press 'Redraw' to update the image!!!



Background Image Island (582 x 519 pixels)

Load Image	Redraw	
Pixel Size (A):	0.165	0.165
Box Size (A):	94	84
Rotation (deg):	2	
Offset (A):	1.5	1.5
Contrast:	0	100

Create Model

Grain:

Tilt (°):

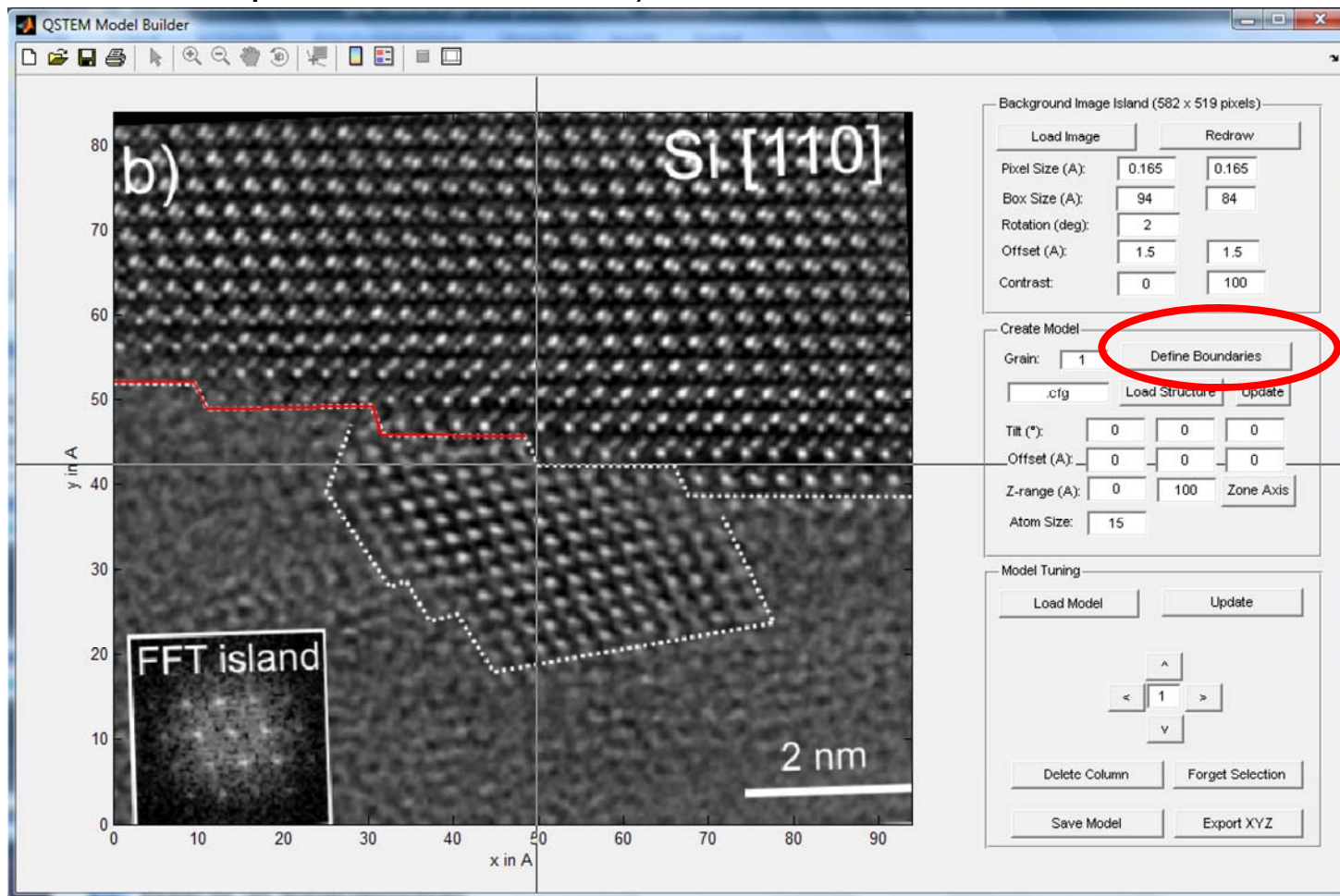
Offset (A):

Z-range (A):

Atom Size:

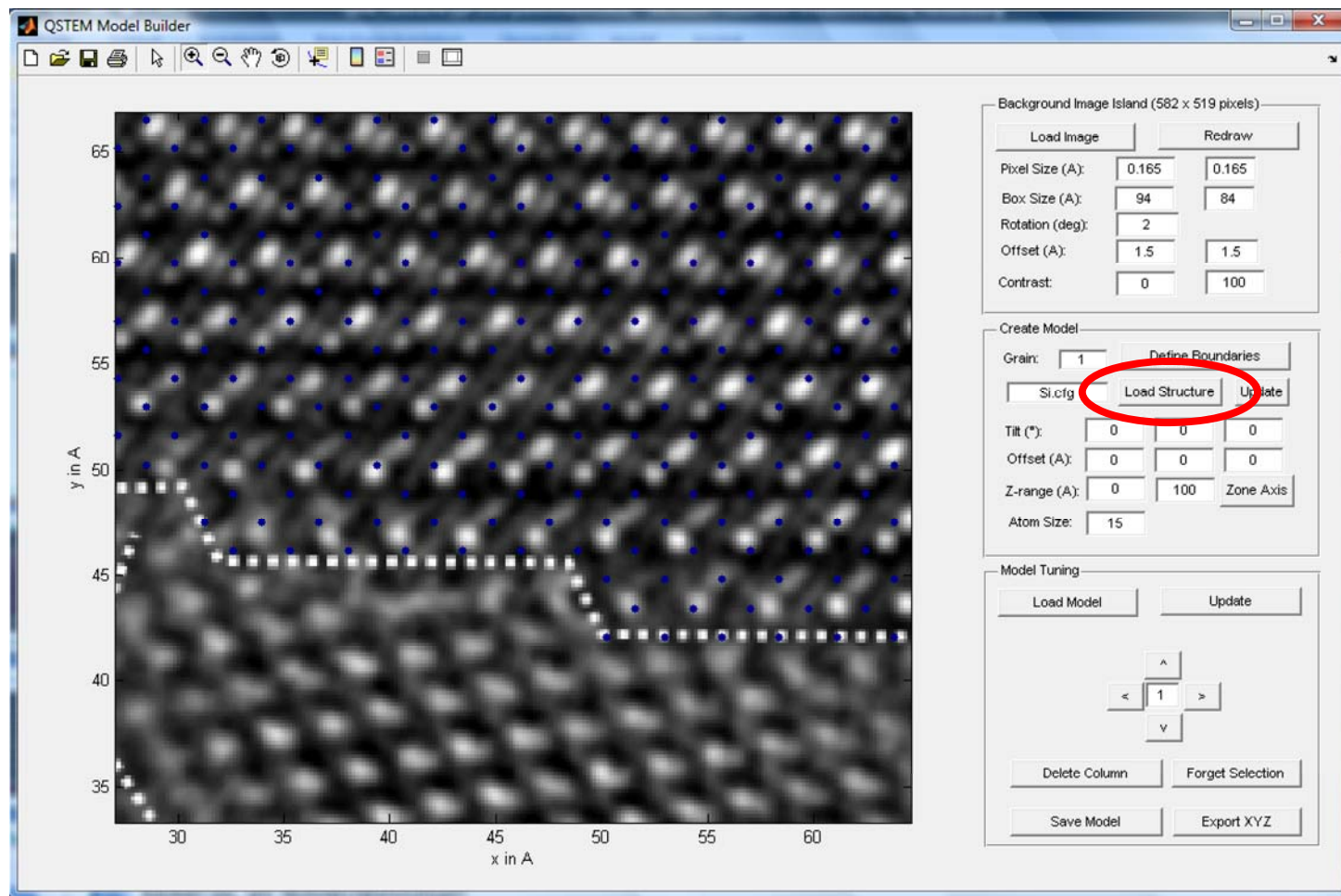
Model Tuning

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)



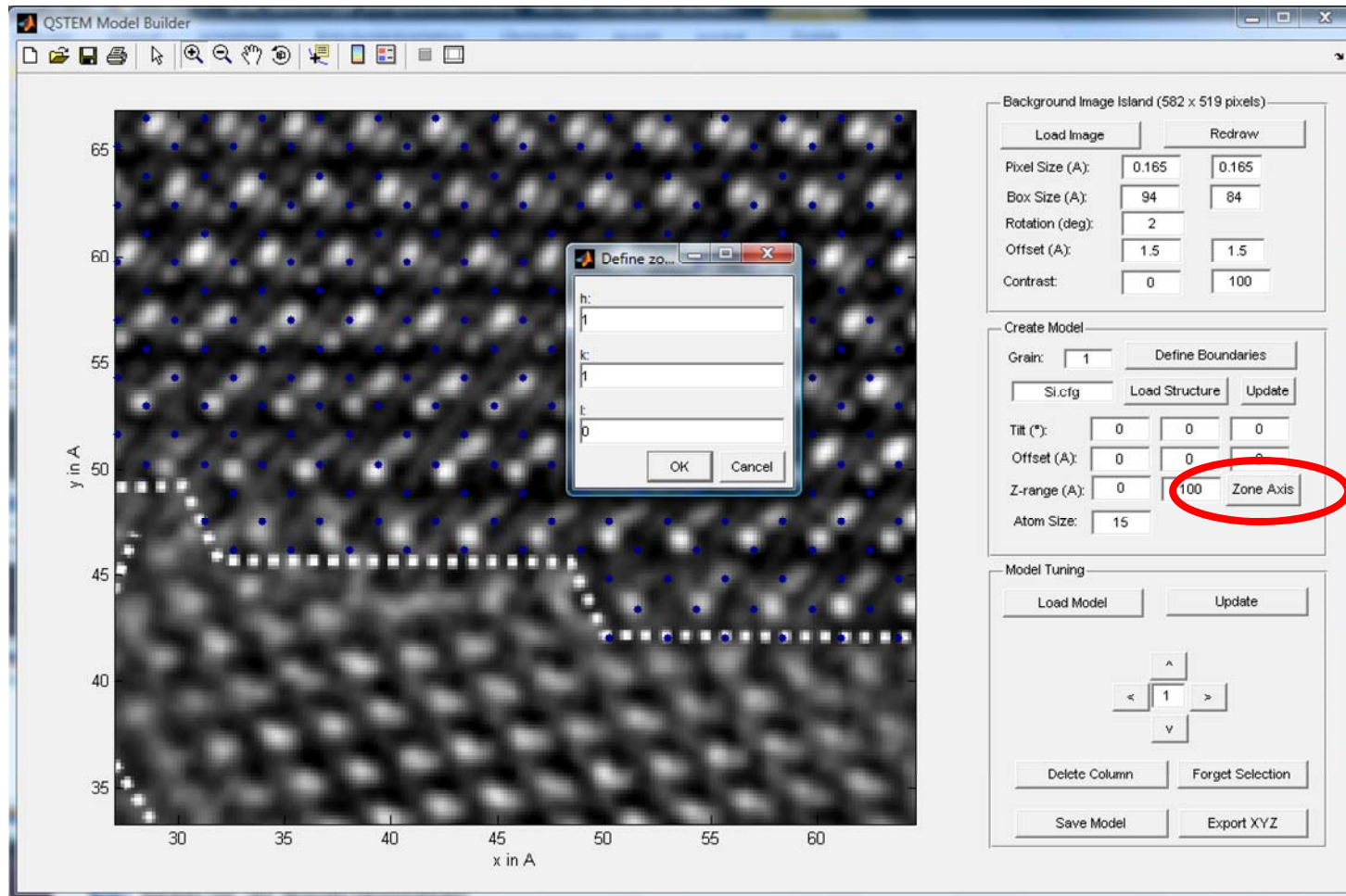


1. Press 'Load Structure' and select the .cfg file you want to fill this grain with (e.g. use Si.cfg from the qmb_Example folder)
2. You may use the toolbar buttons to zoom in/out and pan





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.





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).

QSTEM Model Builder

Background Image Island (582 x 519 pixels)

Load Image Redraw

Pixel Size (A): 0.165 0.165

Box Size (A): 94 84

Rotation (deg): 2

Offset (A): 1.5 1.5

Contrast: 0 100

Create Model

Grain: 1 Define Boundaries

Save Load Update

Tilt (*): 90.000 -45.000 54.1

Offset (A): 1.3 0.9 0

Z-range (A): 0 100 Zone Axis

Atom Size: 25

Model Tuning

Load Model Update

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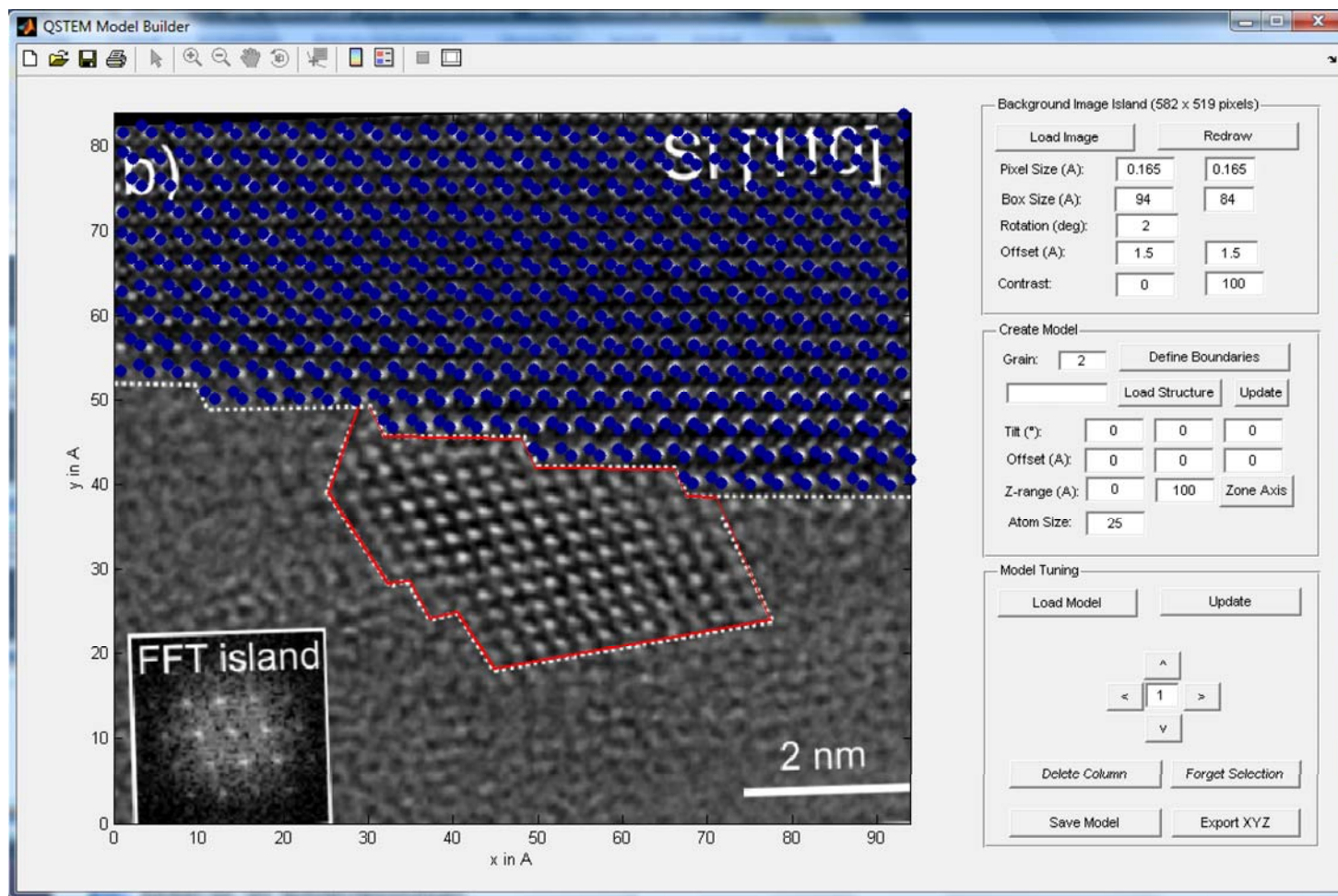
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Delete Column Forget Selection

Save Model Export XYZ

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





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.

QSTEM Model Builder

Background Image Island (582 x 519 pixels)

Load Image Redraw

Pixel Size (A): 0.165 0.165

Box Size (A): 94 84

Rotation (deg): 2

Offset (A): 1.5 1.5

Contrast: 0 100

Create Model

Grain: 2 Define Boundaries

Ti5Si3.cfg Load Structure Update

Tilt (*): -98.790 -23.883 34

Offset (A): 0 -1 0

Z-range (A): 10 90 Zone Axis

Atom Size: 25

Model Tuning

Load Model Update

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Delete Column Forget Selection

Save Model Export XYZ



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.

QSTEM Model Builder

Background Image Island (582 x 519 pixels)

Load Image	Redraw	
Pixel Size (Å):	0.165	0.165
Box Size (Å):	94	84
Rotation (deg):	2	
Offset (Å):	1.5	1.5
Contrast:	0	100

Create Model

Grain: 2 Define Boundaries

Ti5Si3.cfg Load Structure Update

Tilt (°):	-98.790	-23.883	34
Offset (Å):	0	-1	0
Z-range (Å):	10	90	Zone Axis
Atom Size:	25		

Model Tuning

Load Model Update

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Delete Column Forget Selection


Save Model Export XYZ



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

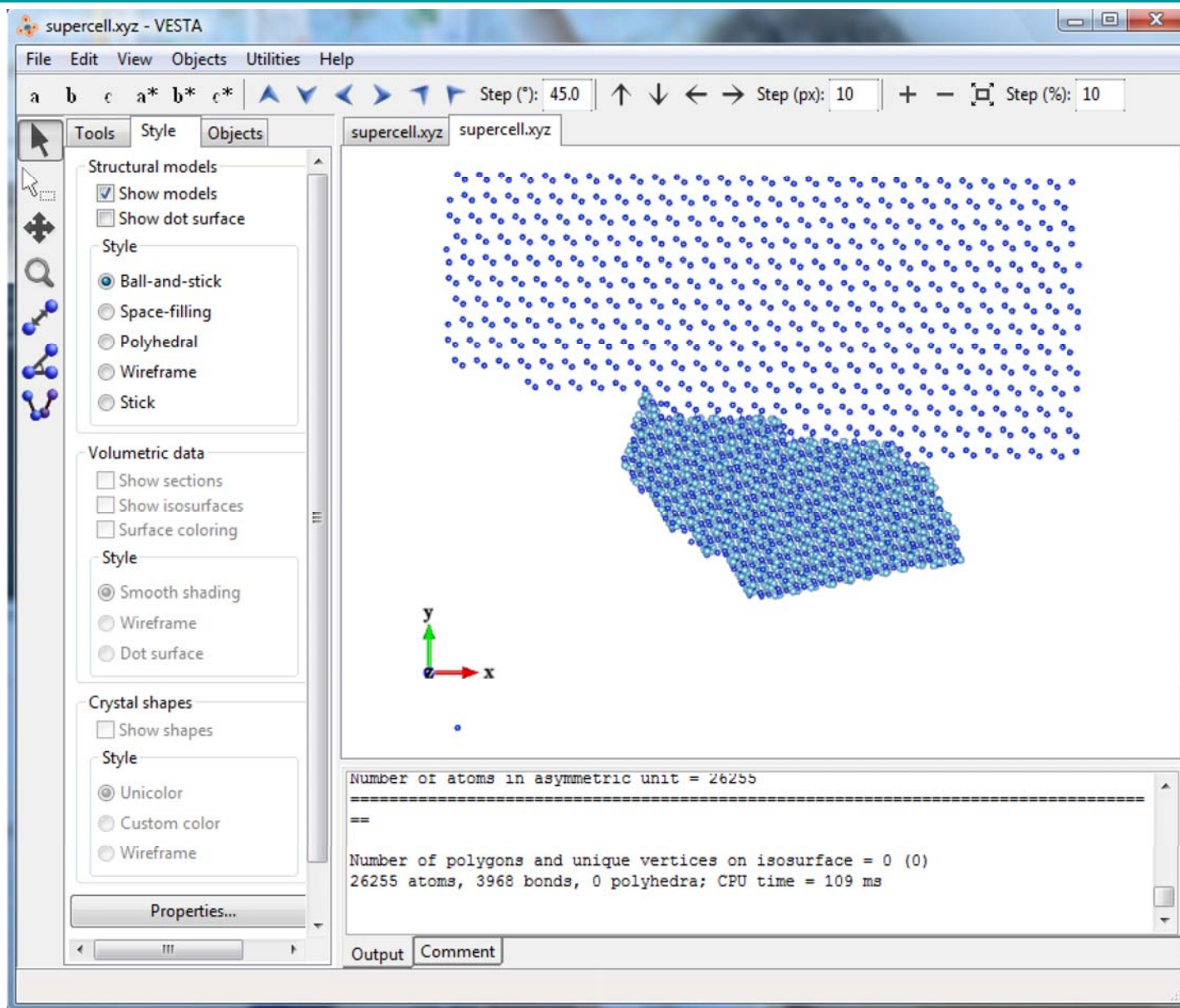
You can export the atomic structure in .xyz format (for display and further processing in other tools*)



Save Model

Export XYZ

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





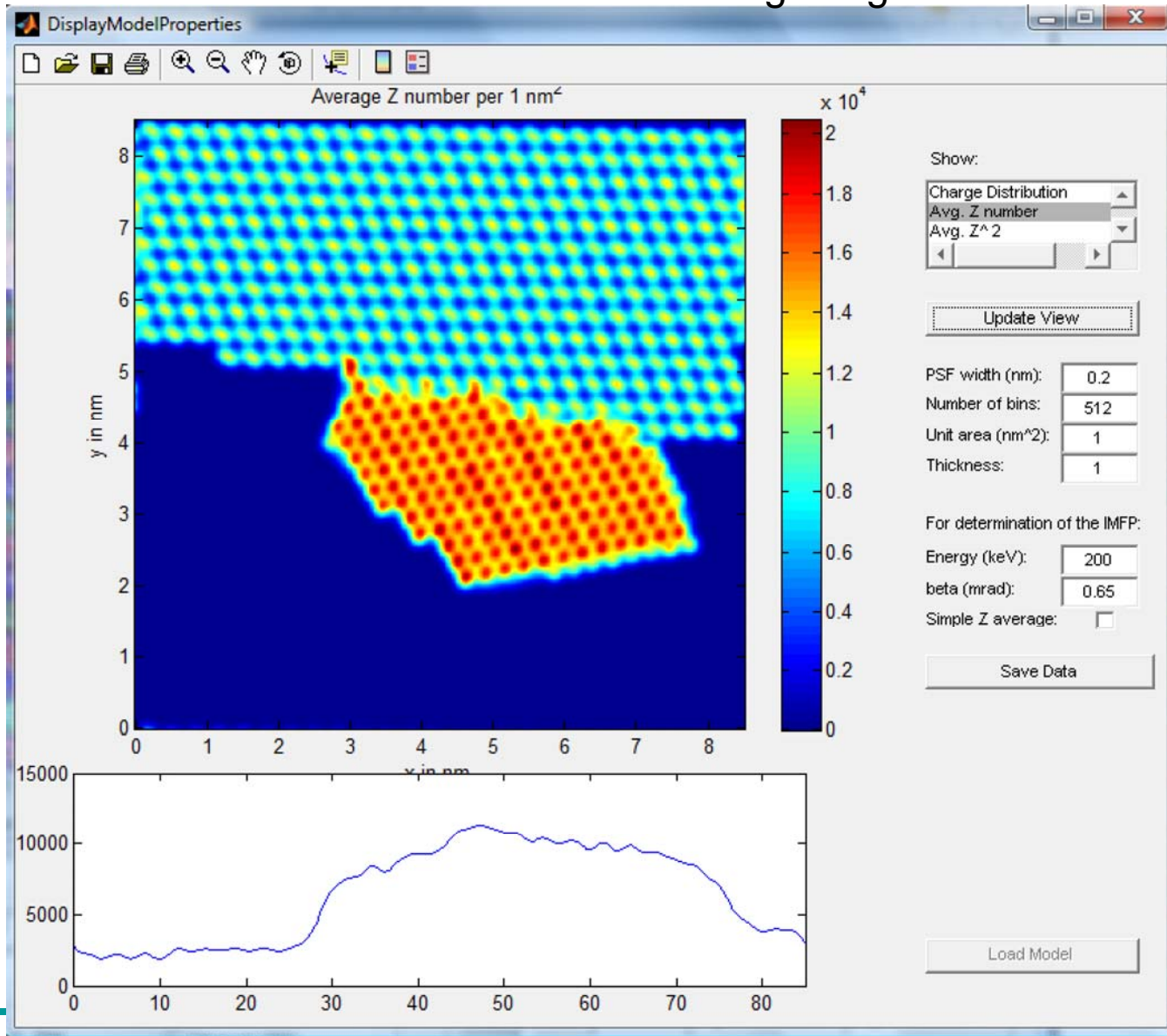
The screenshot displays the qstem software interface. On the left, a 3D visualization shows a model of a Ti5Si3 supercell, represented by blue spheres, set against a light pink background. The axes are labeled from 0 to 80. Below the visualization are controls for loading and updating the model, including a 'Load Model' button and 'Update View' options. The 'Model Properties' section shows 'size' set to 5 and 'Unit cells' (Nx: 1, Ny: 1, Nz: 1). 'Sample tilt' is set to 0 degrees. The 'Simulation mode' is set to TEM.

On the right side, there are several configuration panels:

- Simulate images from wave function**: A button to initiate the simulation.
- Probe array**: Parameters for the probe array, including Array size (400 X 400 pixels), Resolution (0.239438 X 0.213607 A), Window size (95.775 X 85.4426 A), and Scattering angle (34.9 X 39.1 mrad).
- Slicing**: Parameters for the simulation slices, including Number of horizontal model sub-slabs (1), Number of slices per sub-slab (20, Total: 100), and Slice thickness (4.9998 A). It also includes checkboxes for Center slices, Periodic X,Y, and Periodic Z, and Potential offset (X: 0, Y: 0, Z: 0, A: auto z).
- Microscope parameters**: Parameters for the microscope, including High voltage (200 kV, wavelength = 2.51 pm), Defocus (-60 nm, Scherzer), Astigmatism (0 nm, angle: 0 deg), Spherical Aberr. C3 (1.0 mm), Temperature (300 K, TDS runs: 30, checked), Cc (1.0 mm, dE: 0.5 eV), Convergence angle (15 mrad), Beam tilt (X: 0 deg, Y: 0, checked), and Brightness (5 x 10⁸ A/cm2sr, Dwell time: 1 μs).
- Detectors**: Parameters for the detectors, including Number (1), Inner angle (70), Outer angle (200 mrad), and Offset X and Y (0 mrad).
- Output**: Parameters for the output, including Slices between outputs (10) and Folder (test).

At the bottom of the interface, there are buttons for 'Load Config', 'Save Config', 'Advanced Settings', 'Start Simulation', and 'Display Results'.

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



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

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Model: Ti5Si3_Si_superCell_2.cfg

100
90
80
70
60
50
40
30
20
10
0

0 10 20 30 40 50 60 70 80

Load Model Update View 3D Z size View from ...
 Unit cell Slab Super cell top front

Model Properties size 10

Box: ax: 85 by: 85 cz: 99.8477 Box Ncells

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

Simulation mode
 STEM TEM coherent CBED

Load Config Save Config Advanced Settings Start Simulation Display Results

Simulate images from wave function

Probe array
Array size: 512 X 512 pixels
Resolution: 0.166016 X 0.166016 Å
Window size: 85 X 85 Å
Scattering angle: 39.5 X 39.5 mrad

Slicing
Number of horizontal model sub-slabs: 1
Number of slices per sub-slab: 100 (Total: 100)
Slice thickness: 0.9985 Å
 Center slices Periodic X,Y Periodic Z
Potential offset: X: 0 Y: 0 Z: 0 Å auto z

Microscope parameters
High voltage: 300 kV (wavelength = 1.97pm)
Defocus: 3.8 nm Scherzer
Astigmatism: 0 nm, angle: 0 deg
Spherical Aberr. C3: -0.005 mm
Temperature: 300 K, TDS runs: 30 TDS
Cc: 1 mm, dE: 0.5 eV
Convergence angle: 0.3 mrad
Beam tilt: X: 0 deg, Y: 0 tilt back
Brightness (A/cm2sr): 5 x10⁸ Dwell time: 1 µs

Detectors:
Number: 1 Inner angle: 70 Outer angle: 200 mrad
Add Del Offset X: 0 Offset Y: 0 mrad

Output
Slices between outputs: 25 Folder: Particle

TEM Image Formation
- □ X

Real(CTF)

Imag(CTF)

Image t=10.1 nm [0.0000 .. 5.2728]

x in nm

Amorph:	0			
<input checked="" type="checkbox"/> Sampling:	0.0166016	nm		
Acc. Voltage:	300	kV, lambda=0.0197 Å		
<input checked="" type="checkbox"/> Obj. Aperture:	25	mrad	1	mrad
<input type="checkbox"/> Beam Tilt:	0	mrad	0	mrad
<input checked="" type="checkbox"/> Defocus	4.5	nm	Scherzer	
<input checked="" type="checkbox"/> Cs:	-0.007	mm		
<input type="checkbox"/> Astigmatism:	0	nm	0	deg
Defocus step:	0	nm	1	Images
<input type="checkbox"/> Coma:	0	um	0	deg
<input type="checkbox"/> 3-fold Astigm.:	0	um	0	deg
<input checked="" type="checkbox"/> Focal Spread:	3	nm		
<input checked="" type="checkbox"/> Conv. Angle:	0.3	mrad		
<input type="checkbox"/> Pincushion Dist.:	0			
<input type="checkbox"/> Spiral Dist.:	0			
<input type="checkbox"/> Field Curvature:	0			

Update Image

New Figure

Focal Series

Thickn.-Def. Series

Save Wavefunction

Lower Display

Image Diffraction

Amplitude Phase

Upper Display

Wave CTF