Detailed guide on Unit Cell , periodicity and utilities

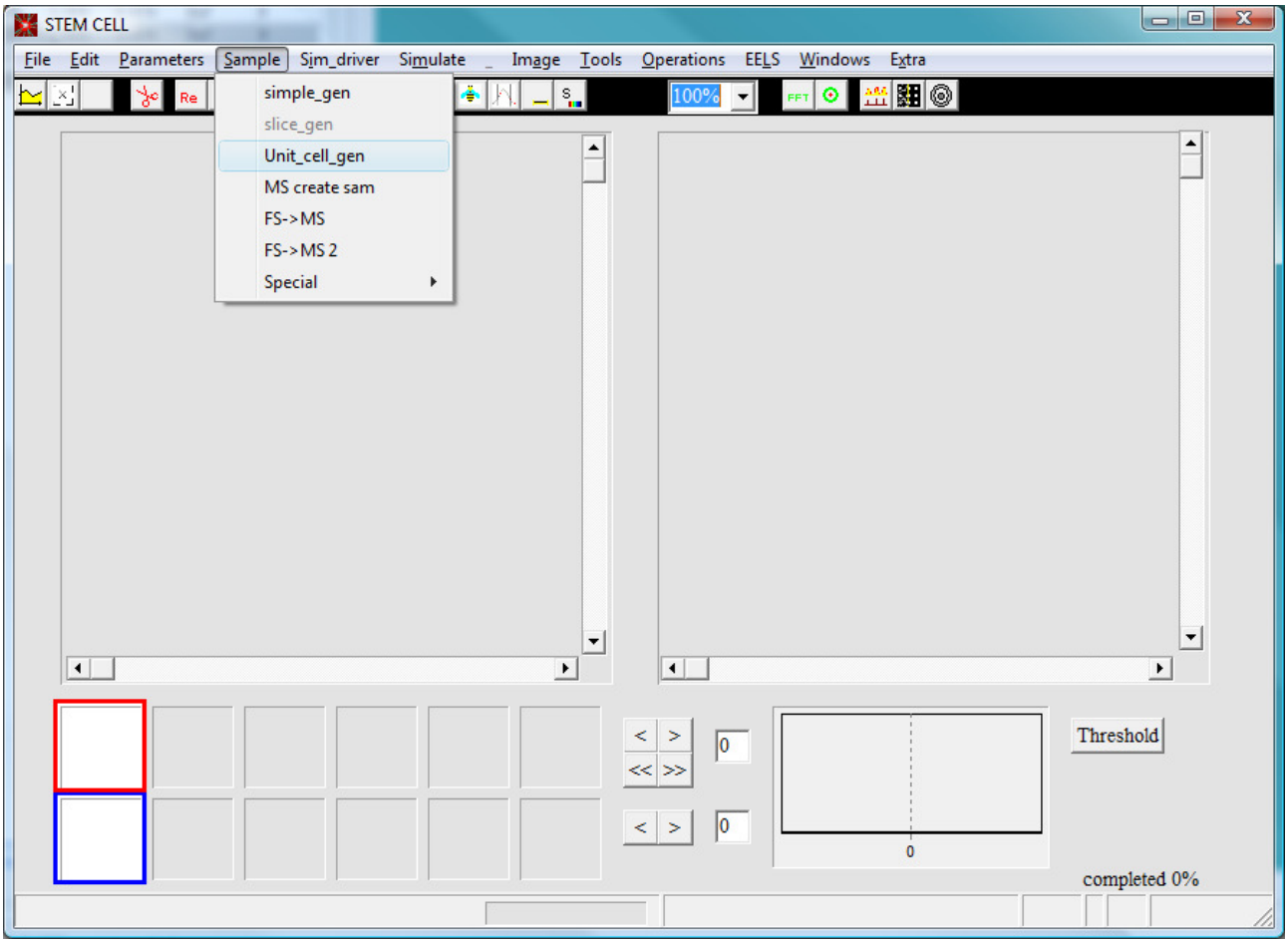
This short guide explains how to create a unit cell and use it in different application

1) For the creation of a supercell
2) To study periodicity and diffraction pattern geometry

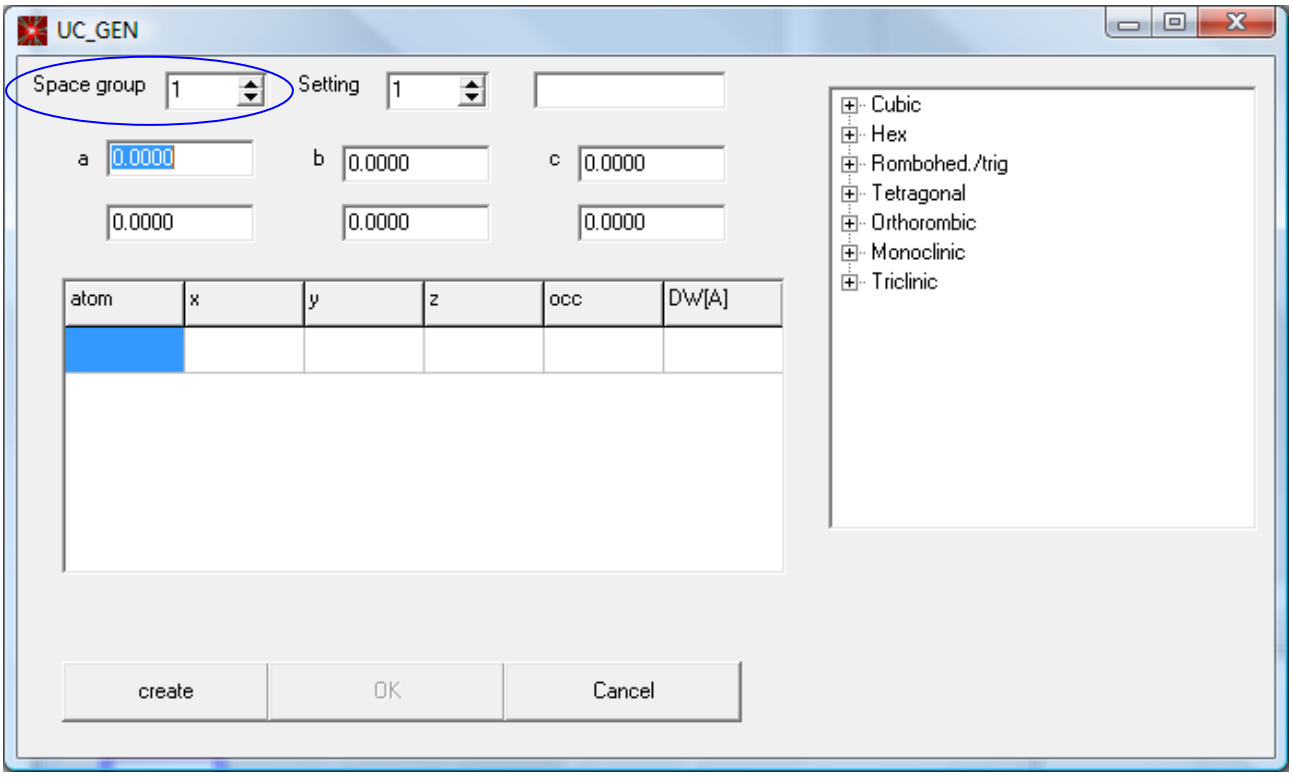
Load and save of the unit cell are also explained

How to create a Unit Cell

Open the unit cell generator



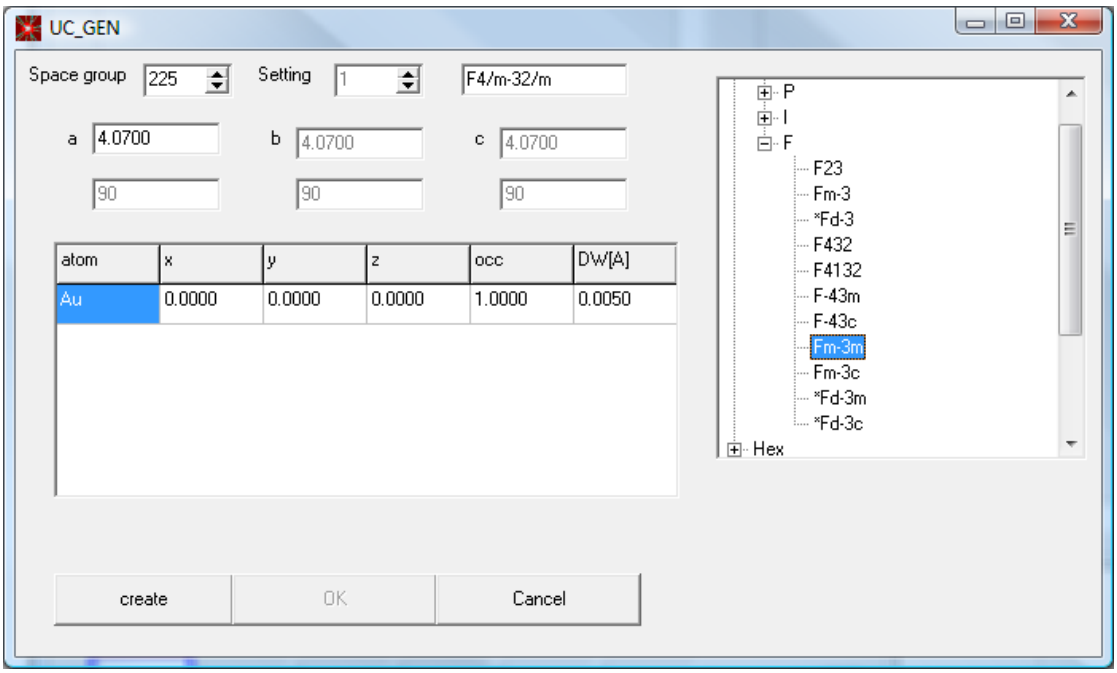
This should open the unit cell creation window



If you know the space group number you can write it in the blue box. You can also specify the setting , you should read the name of the space group in the box on its side.

Alternatively you can browse the desired space group in the right tree (some space group are not implemented at the moment). Double click the group name. This will automatically fill the space group window.

You can then fill the lattice parameters as appropriate (for cubic only one number).

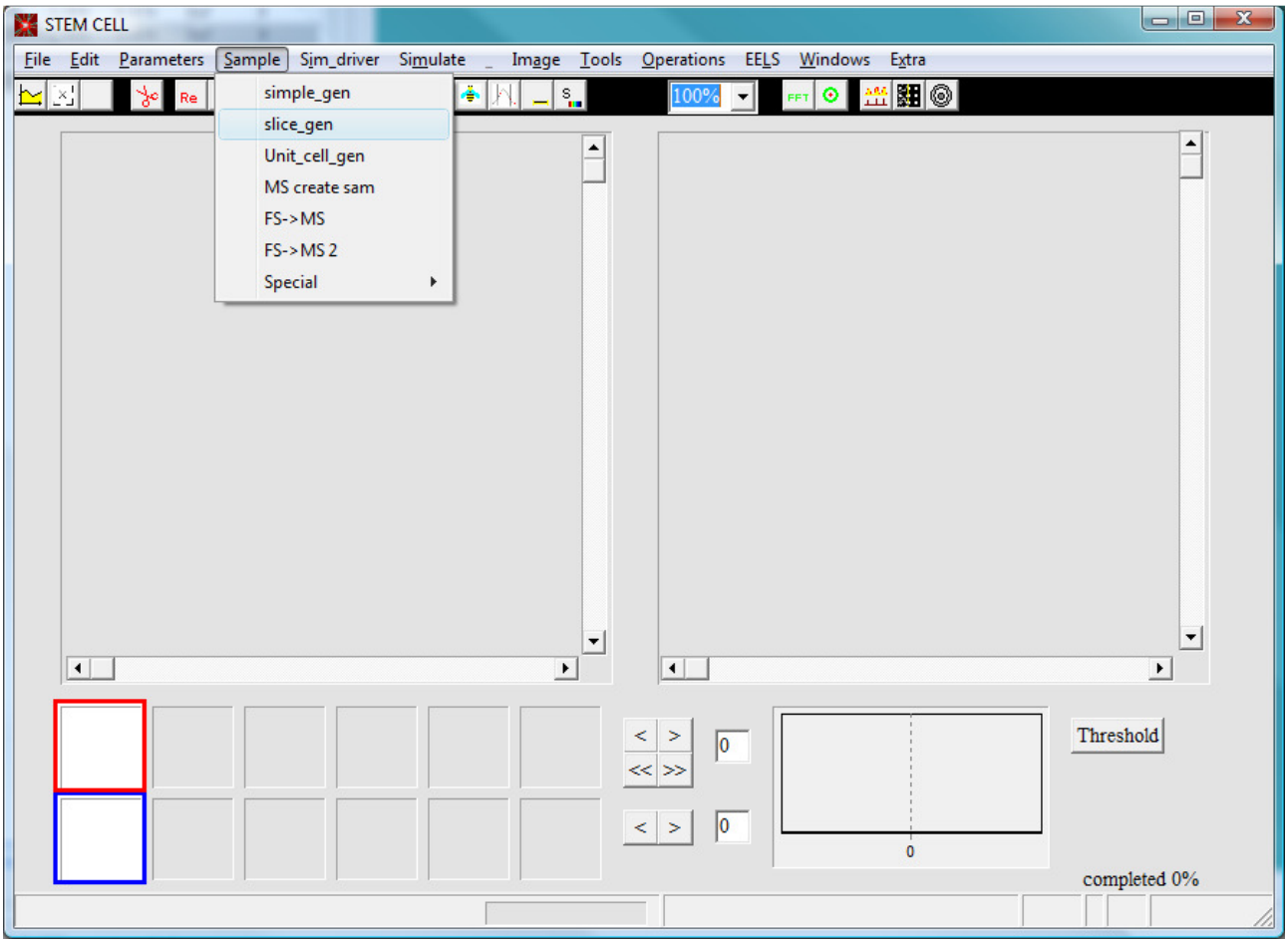


In the example the cell for Au.

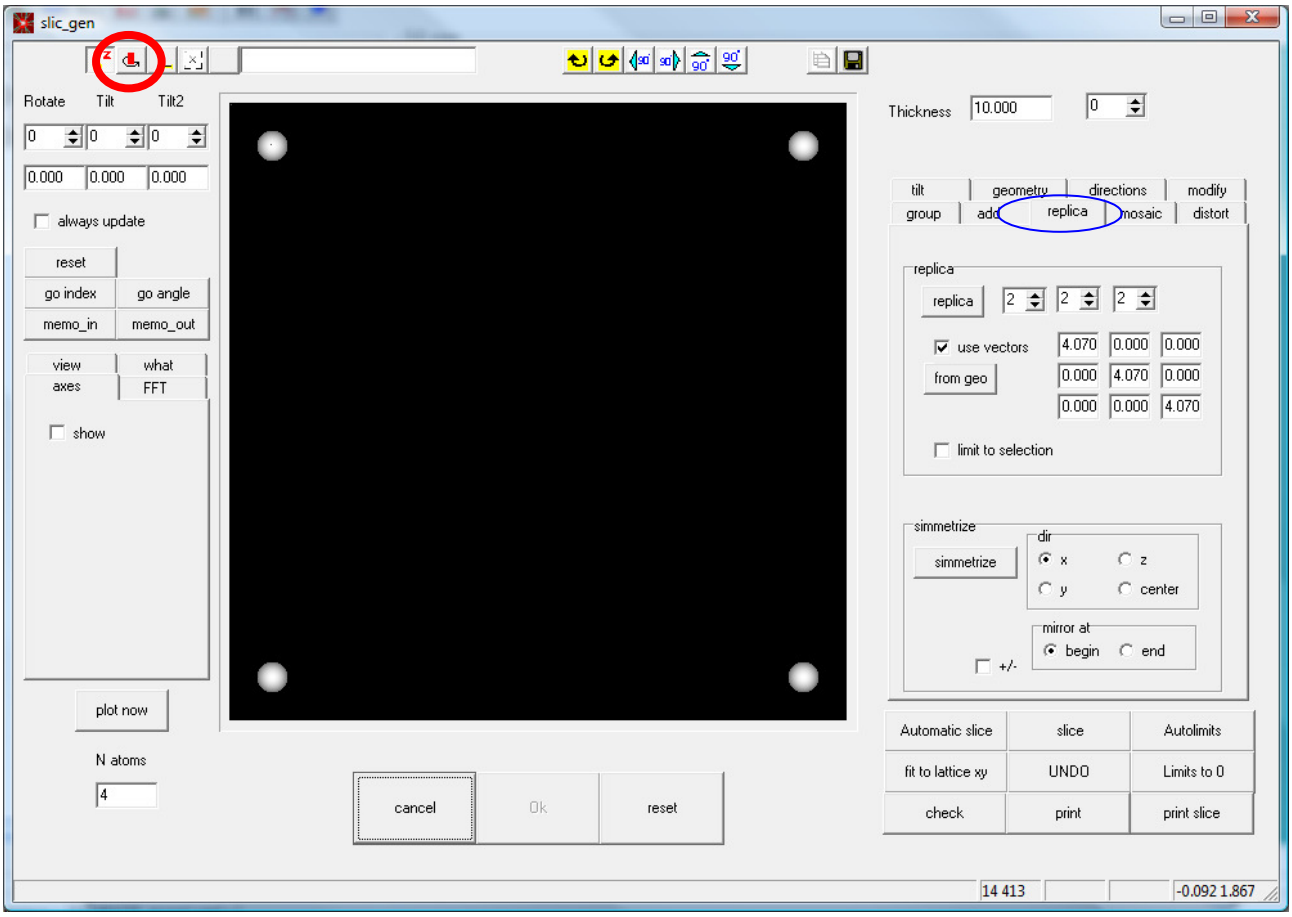
When ready press “create” this will create the cell and also a supercell (SC) based on this(in future version the SC creation will have a separate button). Close the window

A quick look at the cell

It can be interesting to take a look at the unit cell. Let ‘s go then at



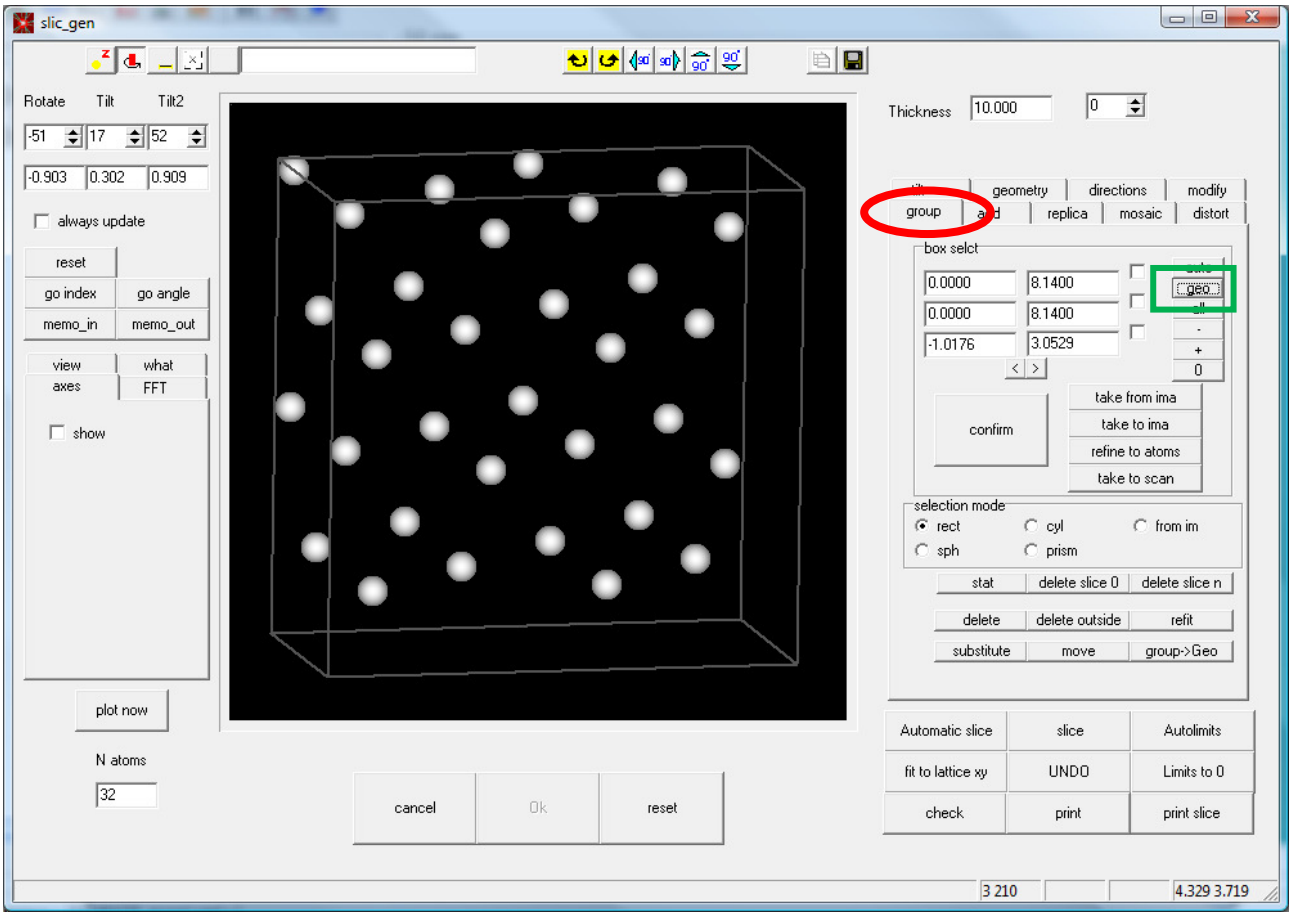
This will show the 4 basis atom as follows



For a better visualisation we can duplicate the basis at least once.

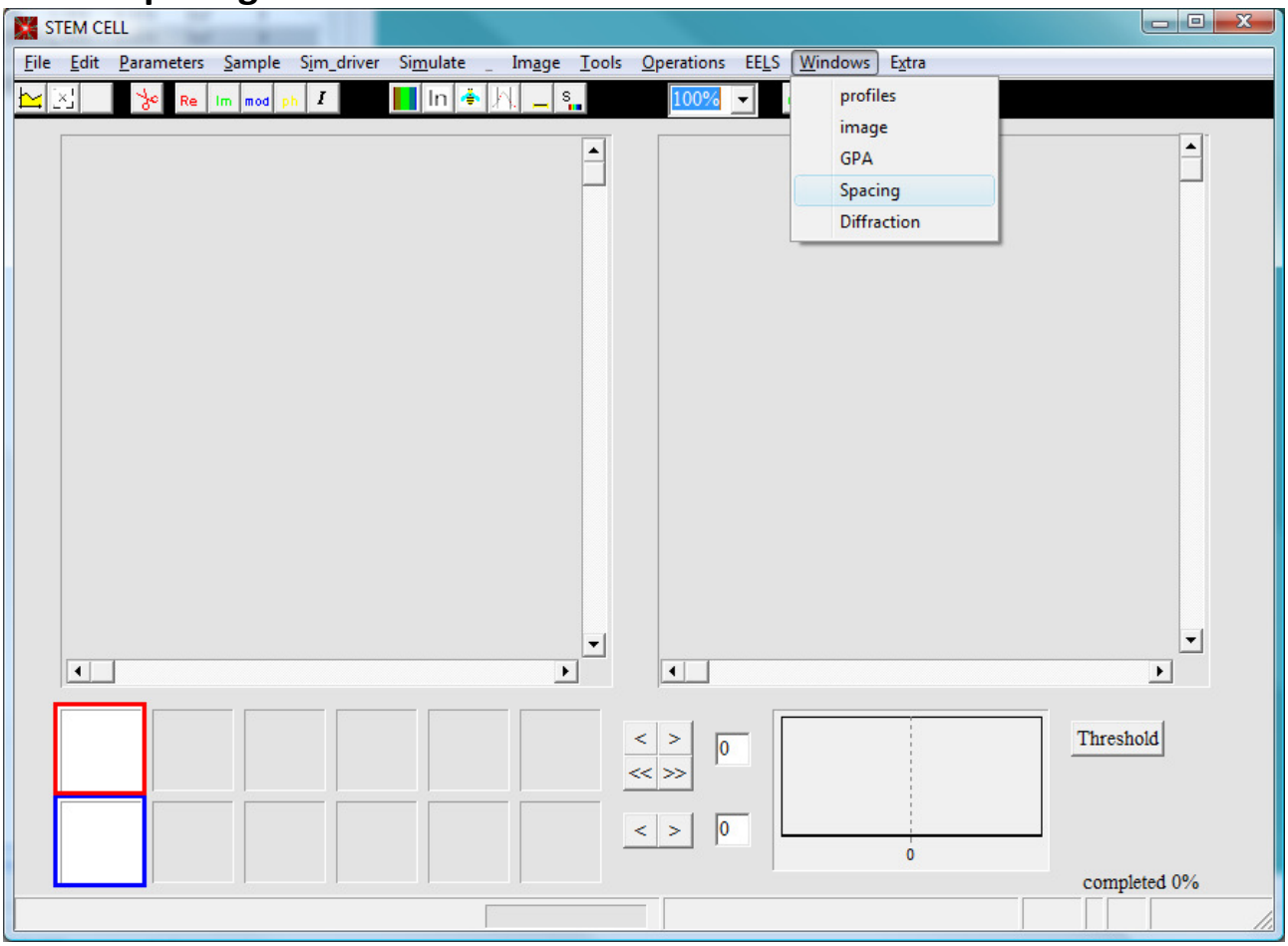
Press the Replica Tab and select 2,2,2 (the default)

Pres then the button here in red to activate the drag and drop rotation of the cell



We can also be helped by selecting the group TAB and pressing GEO. This will highlight a rectangular prism containing the cell. This unit is usefull for many supercell manipulation but is not the topic of this description.

Lattice spacings



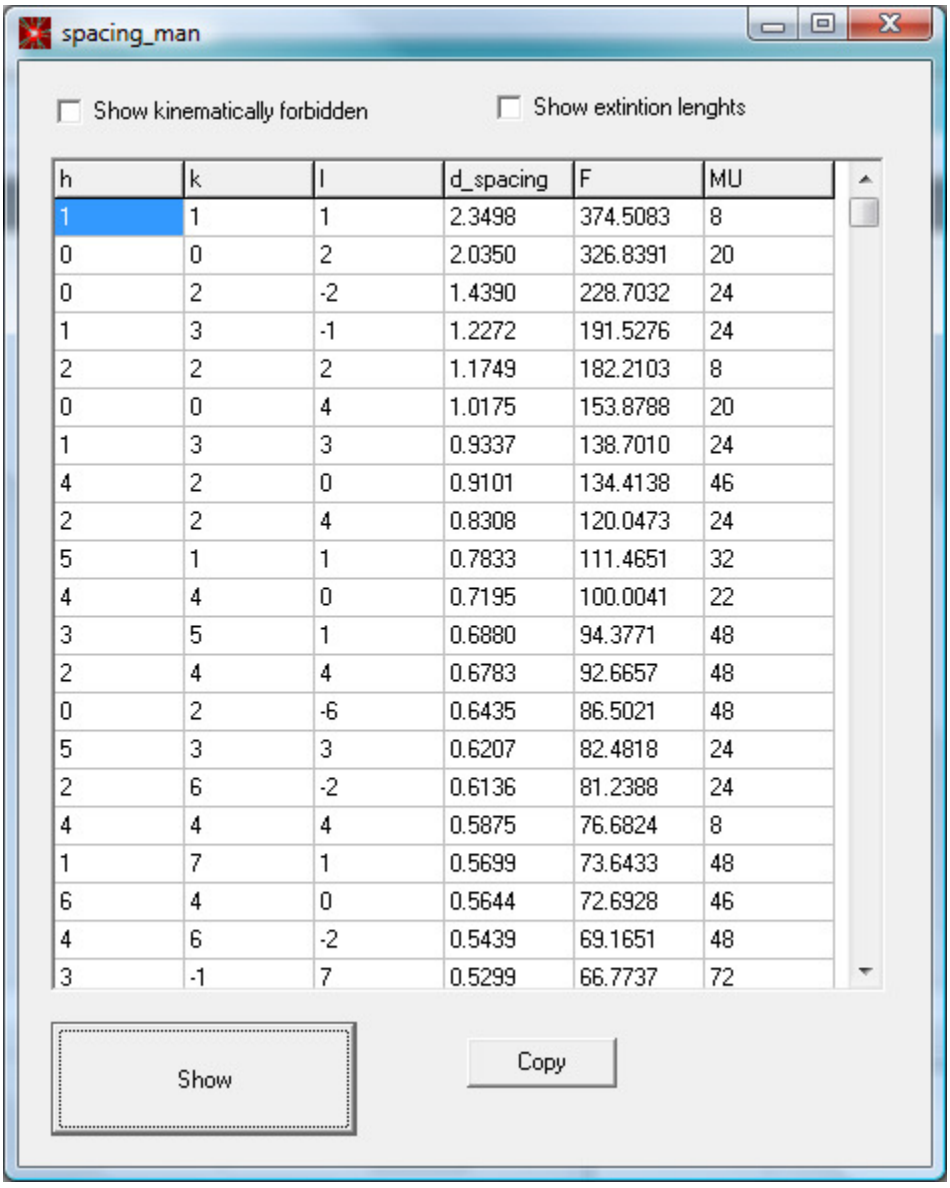
Open the spacing window. When it opens press the button “show”.

The reflection with the d-spacing should appear. Also scattering factor F and multiplicity MU should appear.

By checking tehappropriate box you can visualize also kinematically frobidedn reflection and the extension distance instead of F.

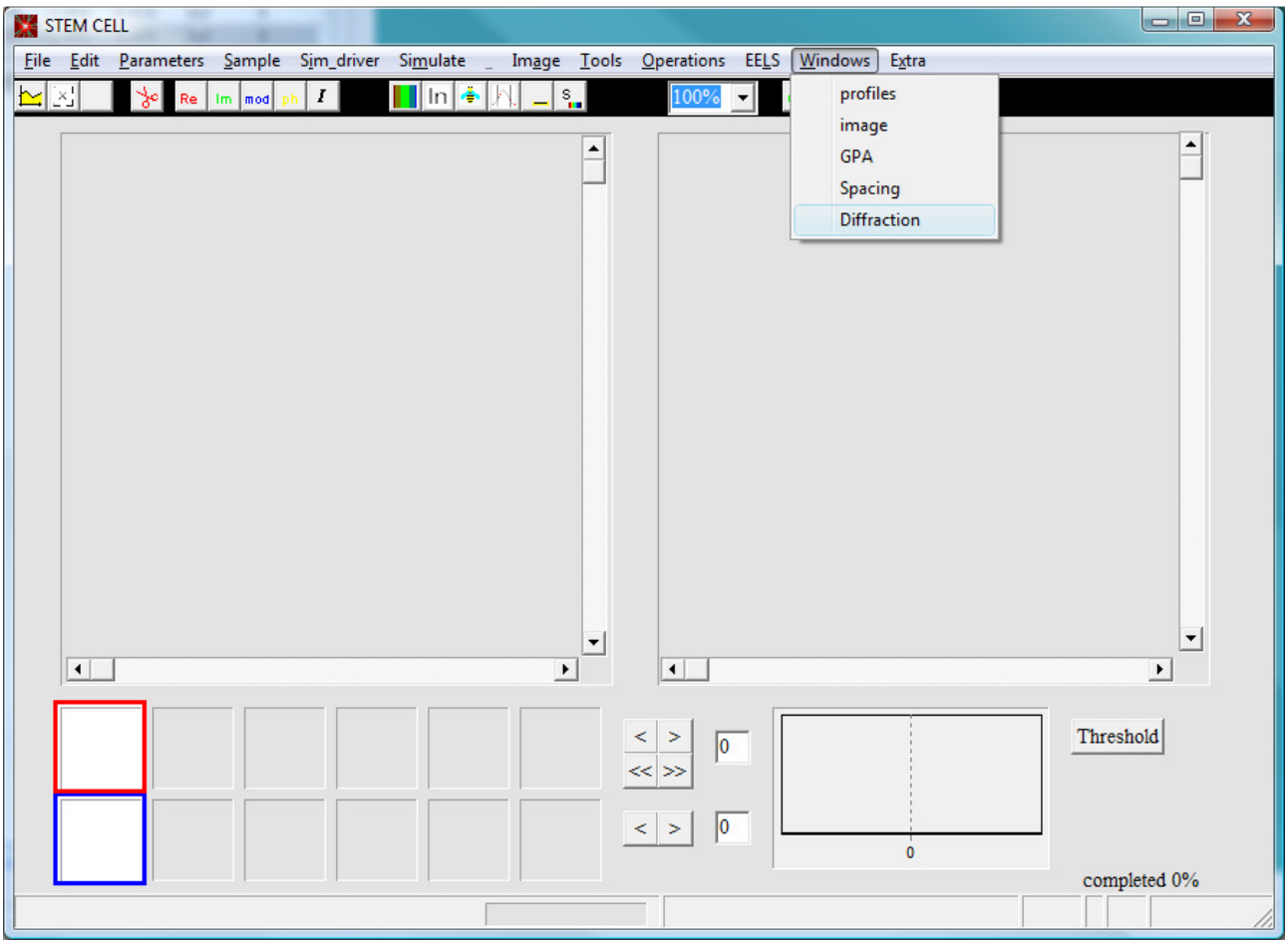
From version 2.3.6.6 another button permits to copy on clipboard (and then paste on MS word) a summarization of reflection and lattice distances.

Close it when ready.


spacing_man
Show kinematically forbidden
Show extintion lenghts
h k l d_spacing F MU
1 1 1 2.3498 374.5083 8
0 0 2 2.0350 326.8391 20
0 2 -2 1.4390 228.7032 24
1 3 -1 1.2272 191.5276 24
2 2 2 1.1749 182.2103 8
0 0 4 1.0175 153.8788 20
1 3 3 0.9337 138.7010 24
4 2 0 0.9101 134.4138 46
2 2 4 0.8308 120.0473 24
5 1 1 0.7833 111.4651 32
4 4 0 0.7195 100.0041 22
3 5 1 0.6880 94.3771 48
2 4 4 0.6783 92.6657 48
0 2 -6 0.6435 86.5021 48
5 3 3 0.6207 82.4818 24
2 6 -2 0.6136 81.2388 24
4 4 4 0.5875 76.6824 8
1 7 1 0.5699 73.6433 48
6 4 0 0.5644 72.6928 46
4 6 -2 0.5439 69.1651 48
3 -1 7 0.5299 66.7737 72
Show
Copy

Diffraction

Press window-> diffarction



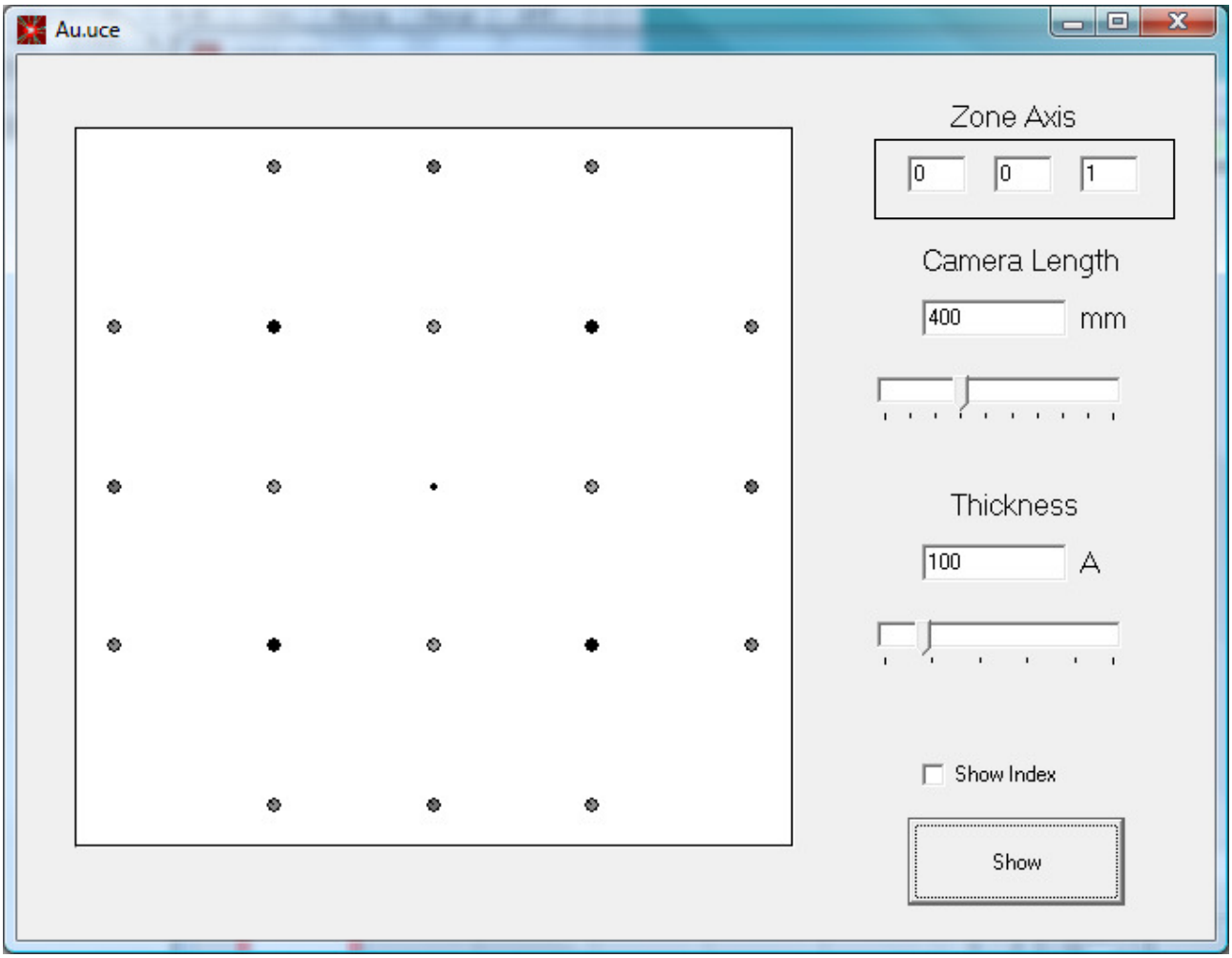
In this way a diffraction windows appears.

The most important number her below indicated by a rectangle can be set to define the zone axis to be visualized.

The camera Length permits to zoom the pattern (use the scroll).

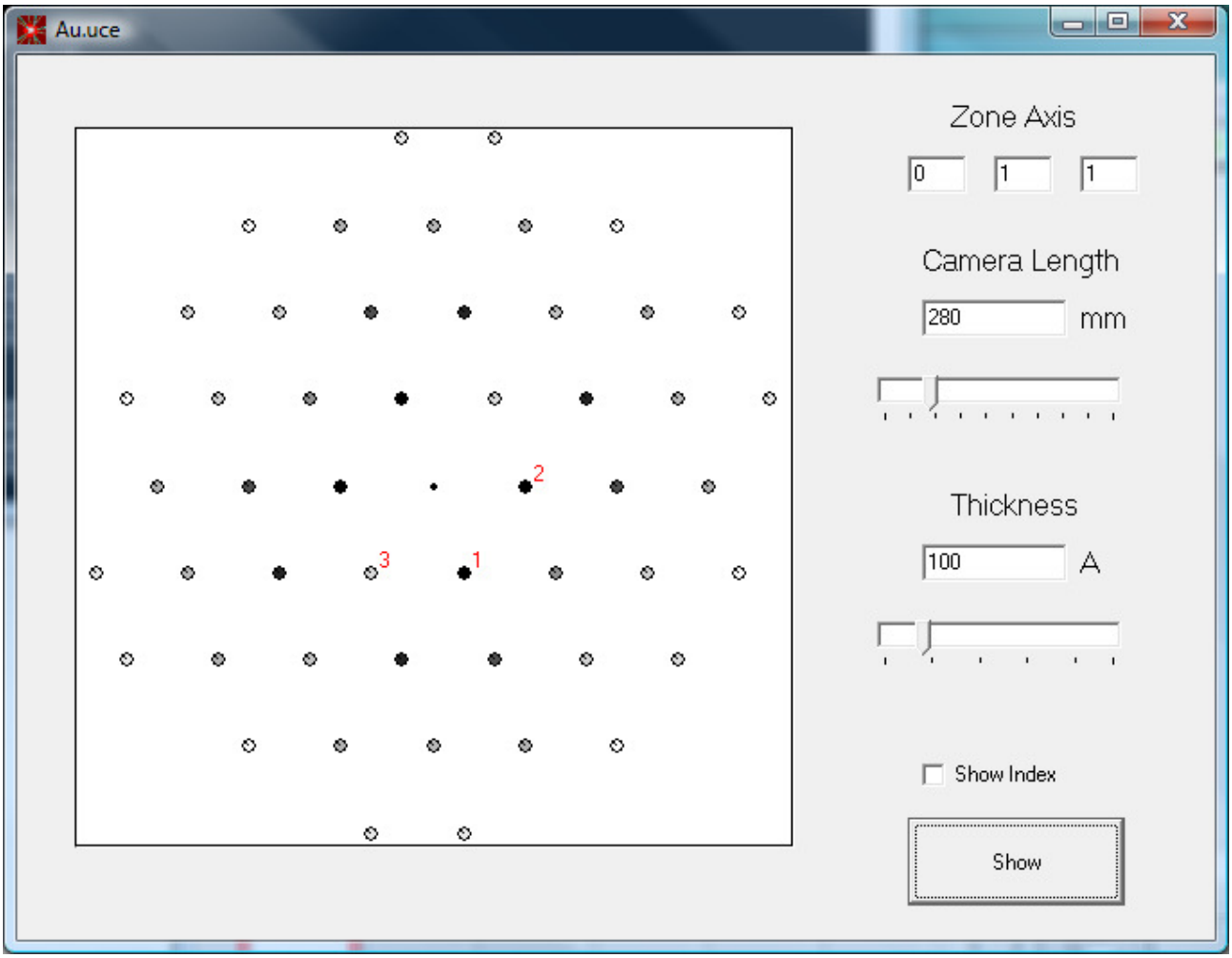
By changing the thickness the intensity of the spot is estimated by 2 beam diffraction equation.

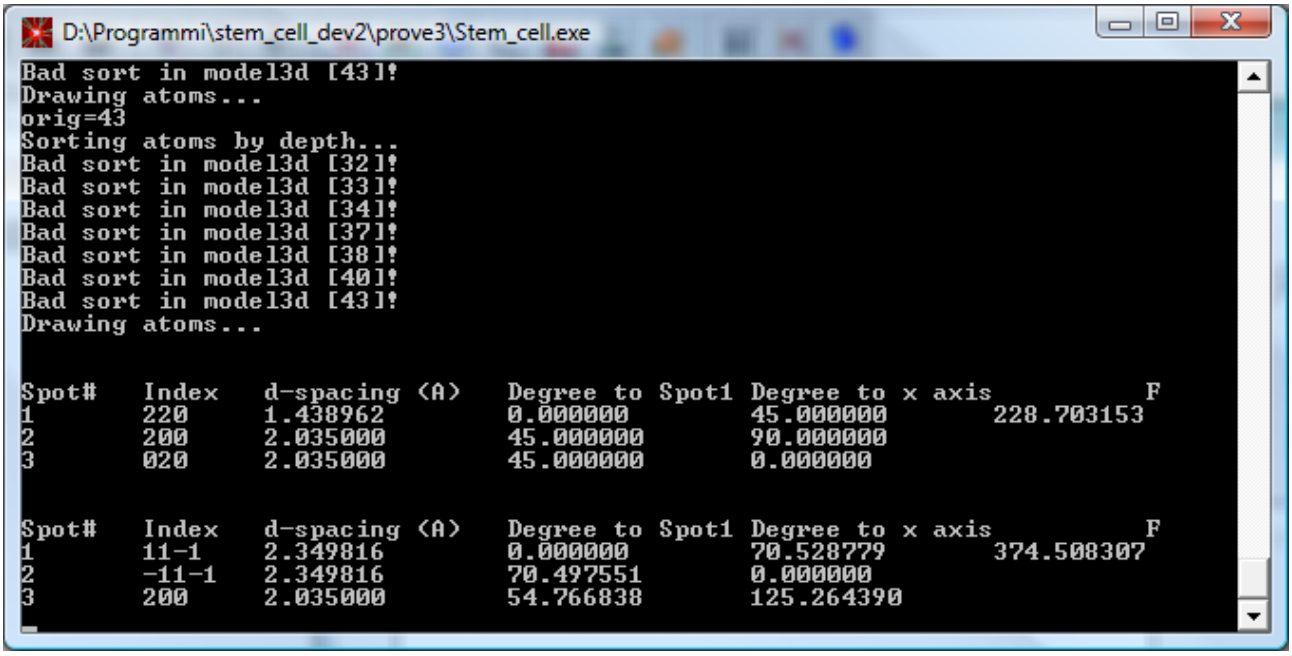
If you thick the “show index2 box and “show2 you can visualize the index of the reflections.



IMPORTANT utility

If you click on a single reflection a number appears on it. Now if you look at the debug window you should see the index name and the relative angle between numbered spots.


Au.uce
Zone Axis
0
1
1
Camera Length
280
mm
Thickness
100
A
Show Index
Show
1
2
3


D:\Programmi\stem_cell_dev2\prove3\Stem_cell.exe
Bad sort in model3d [43]!
Drawing atoms...
orig=43
Sorting atoms by depth...
Bad sort in model3d [32]!
Bad sort in model3d [33]!
Bad sort in model3d [34]!
Bad sort in model3d [37]!
Bad sort in model3d [38]!
Bad sort in model3d [40]!
Bad sort in model3d [43]!
Drawing atoms...
Spot# Index d-spacing (A) Degree to Spot1 Degree to x axis F
1 220 1.438962 0.000000 45.000000 228.703153
2 200 2.035000 45.000000 90.000000
3 020 2.035000 45.000000 0.000000
Spot# Index d-spacing (A) Degree to Spot1 Degree to x axis F
1 11-1 2.349816 0.000000 70.528779 374.508307
2 -11-1 2.349816 70.497551 0.000000
3 200 2.035000 54.766838 125.264390