

## Detailed guide on Unit Cell , periodicity and utilities

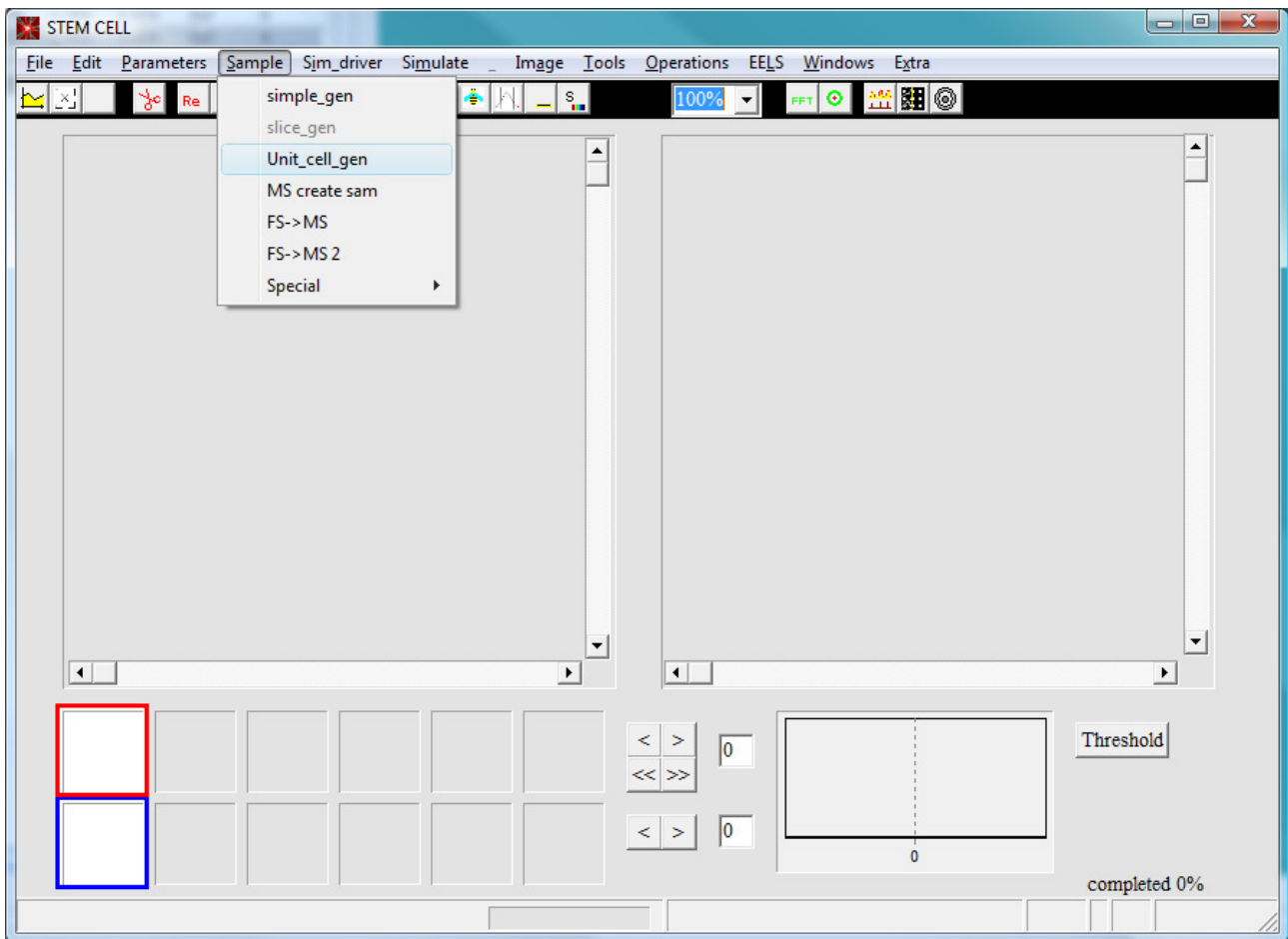
This short guide explains how to create a unit cell and use it in different application

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

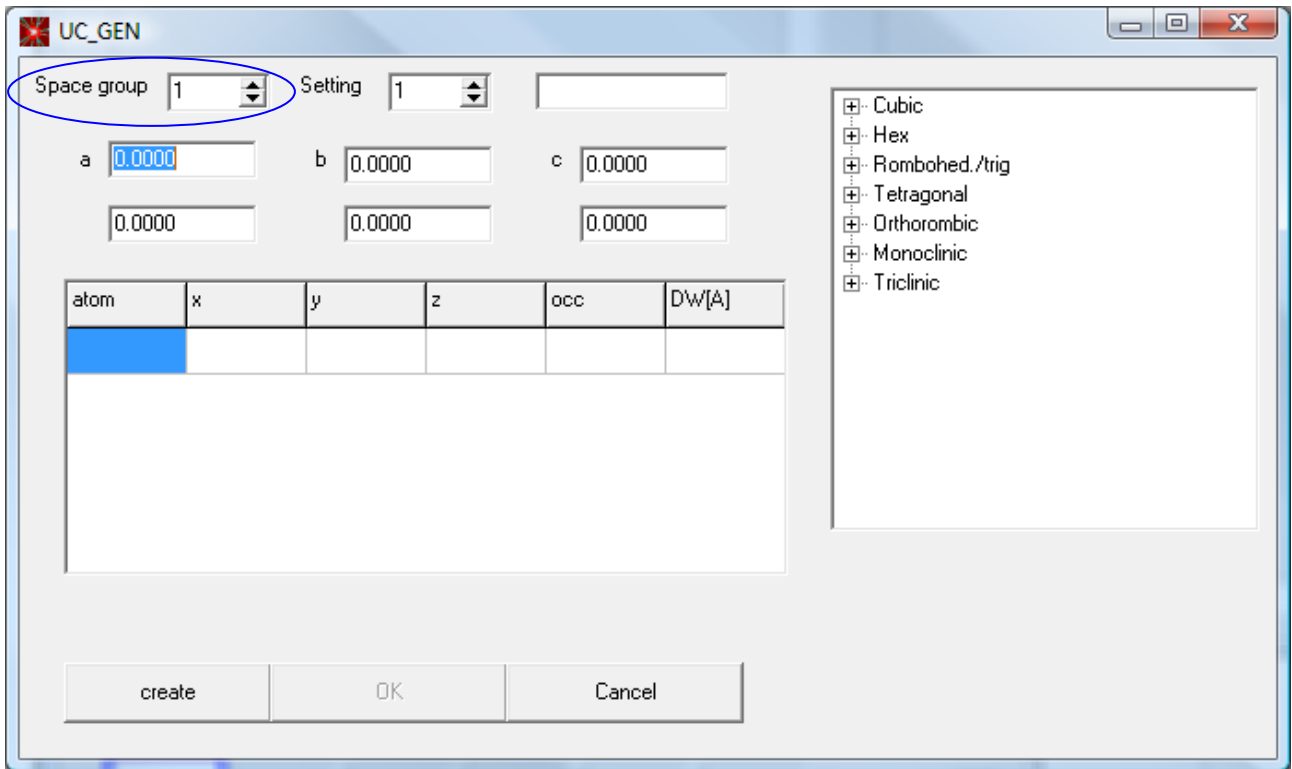
Load and save of the unit cell are also explained

### How to create a Unit Cell

Open the unit cell generator



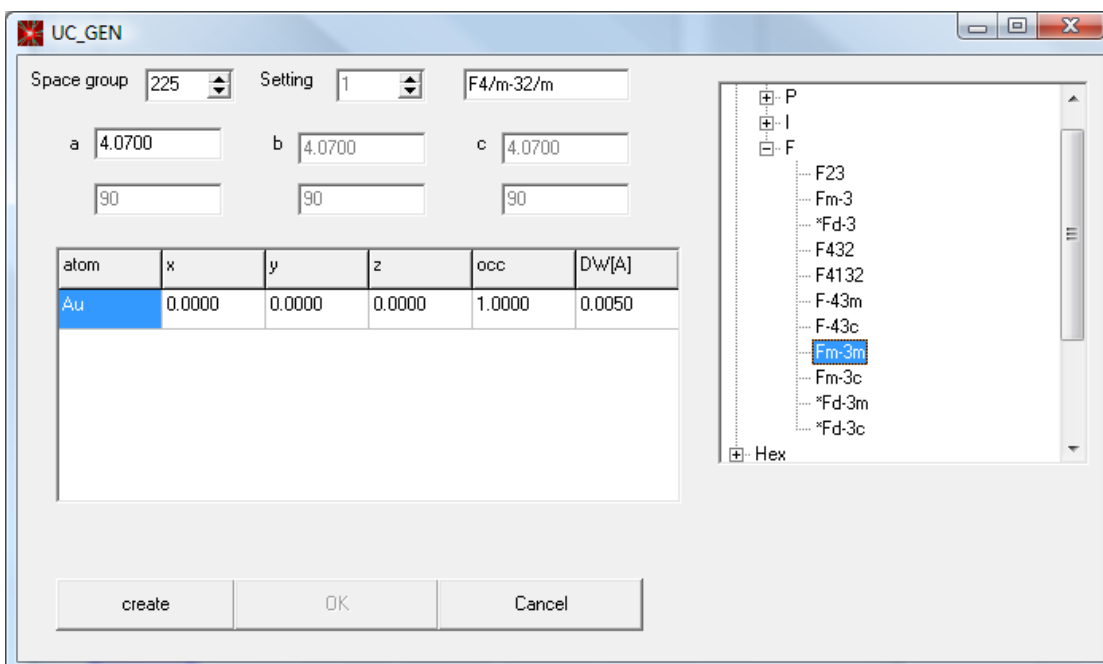
This should open the unit cell creation window



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 groups 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).

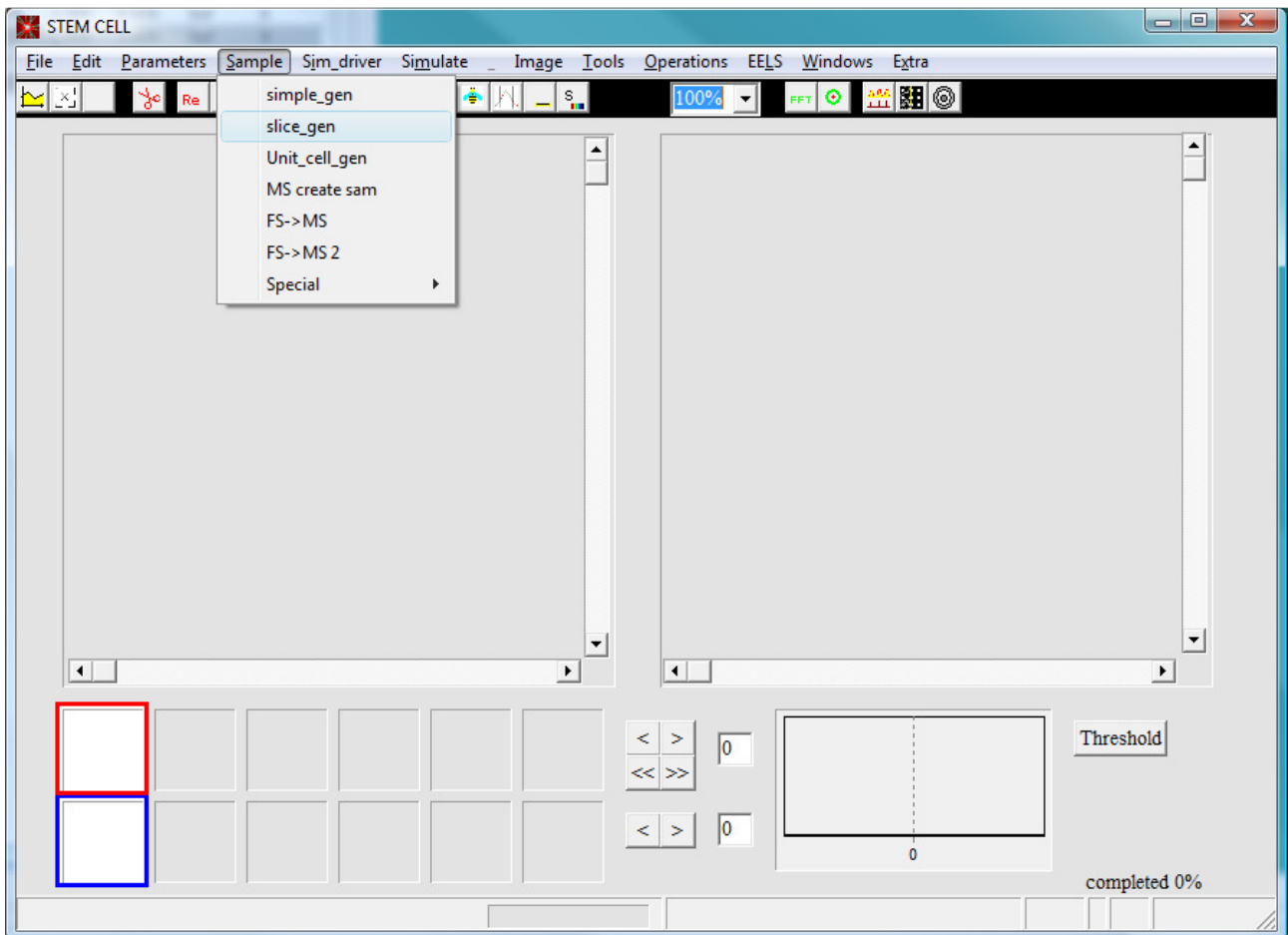


In the example the cell for Au.

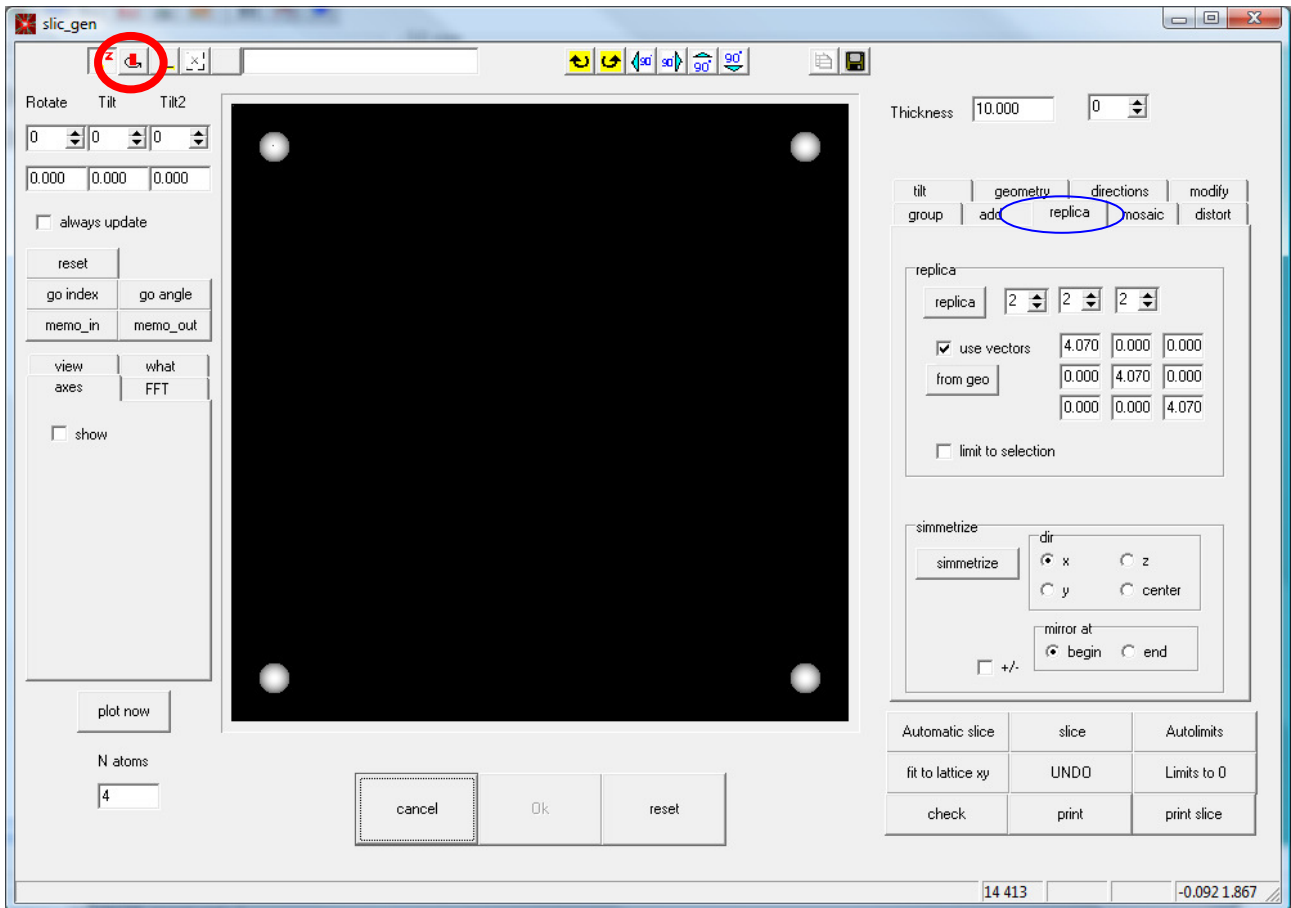
When ready press “create” this will create the cell and also a supercell (SC) based on this( in future version the SC creation will have a separate button). Close the window

### A quick look at the cell

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



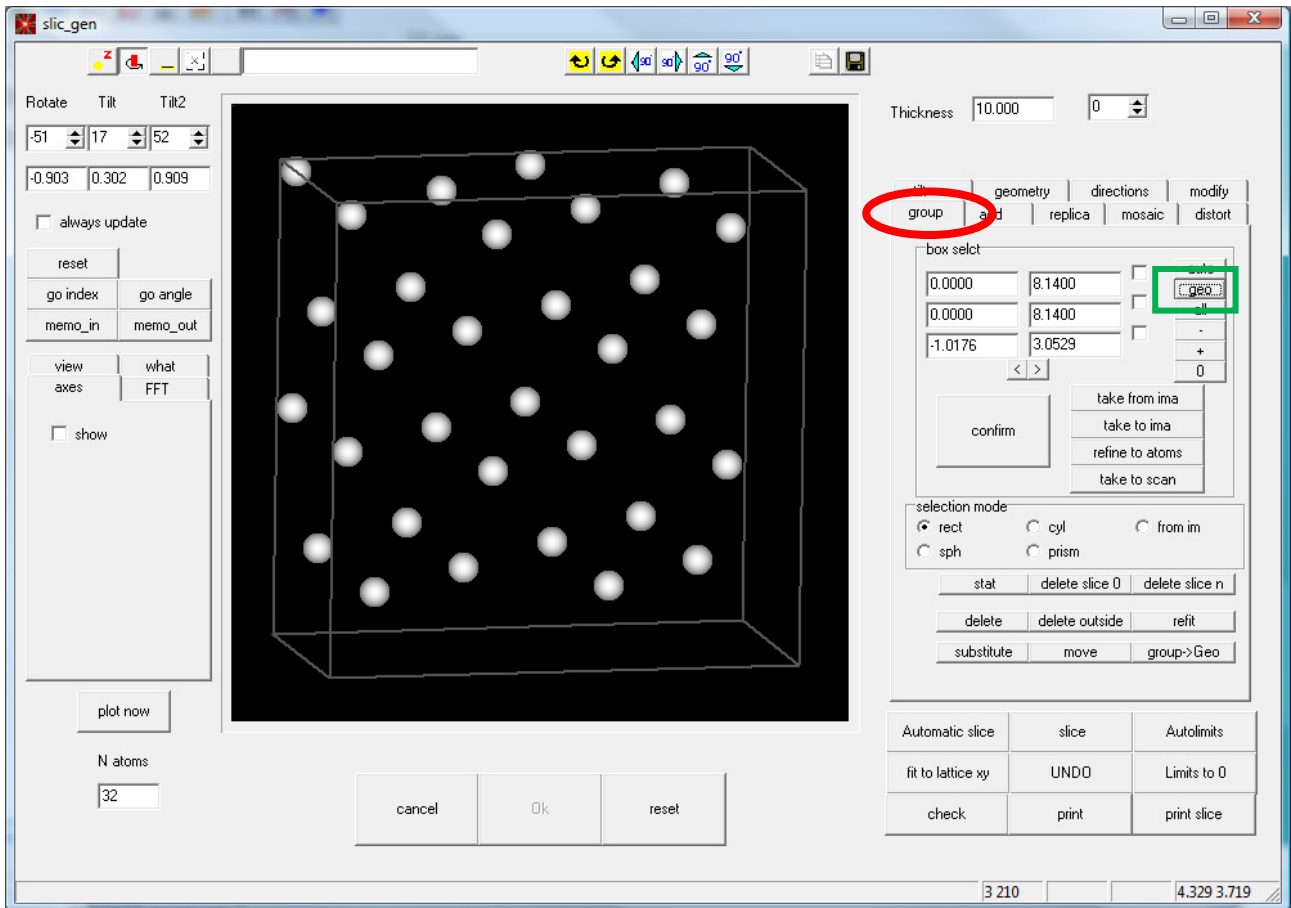
This will show the 4 basis atom as follows



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

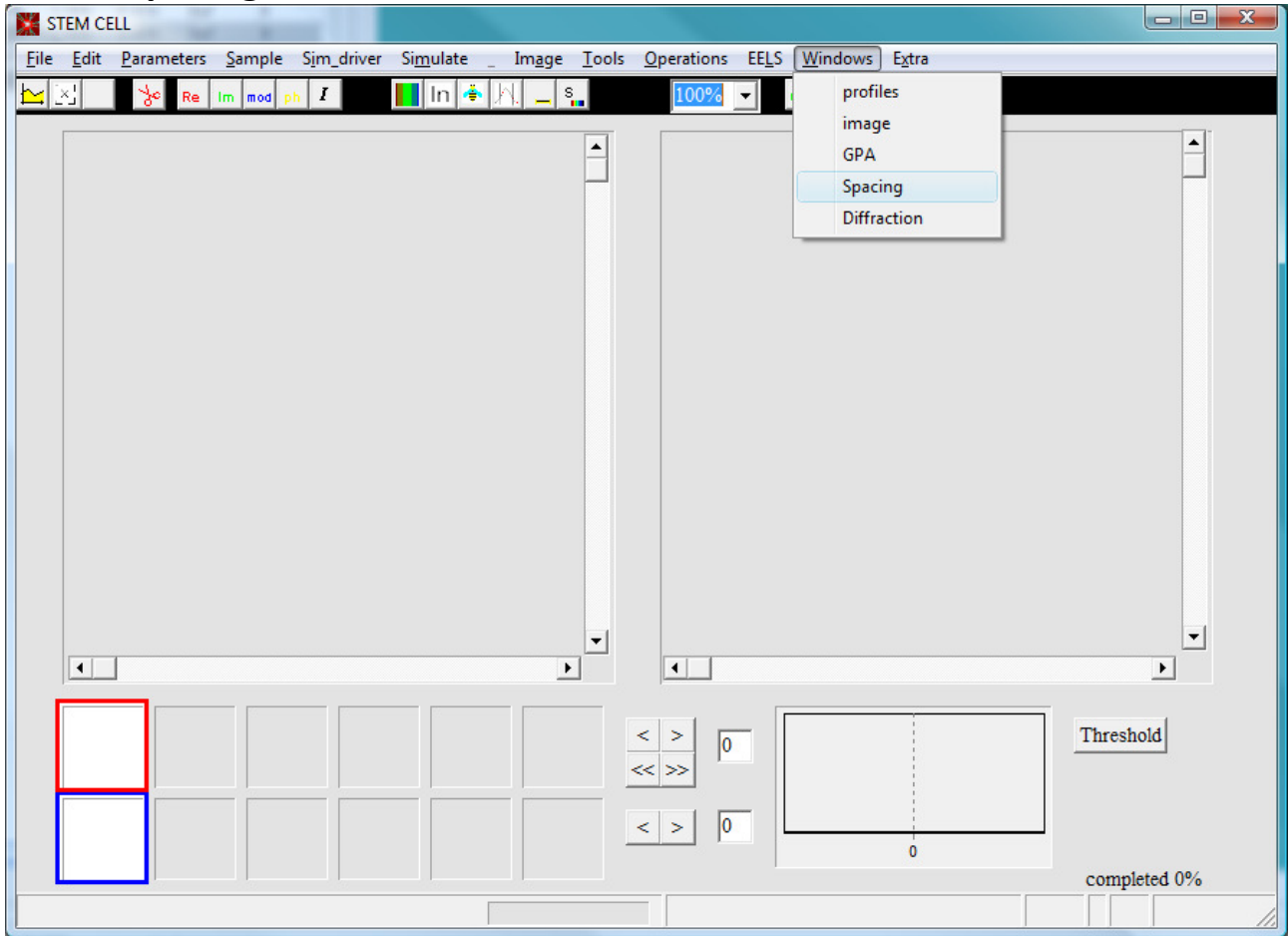
Press the Replica Tab and select 2,2,2 ( the default )

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 useful 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 the appropriate box you can visualize also kinematically forbidden 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

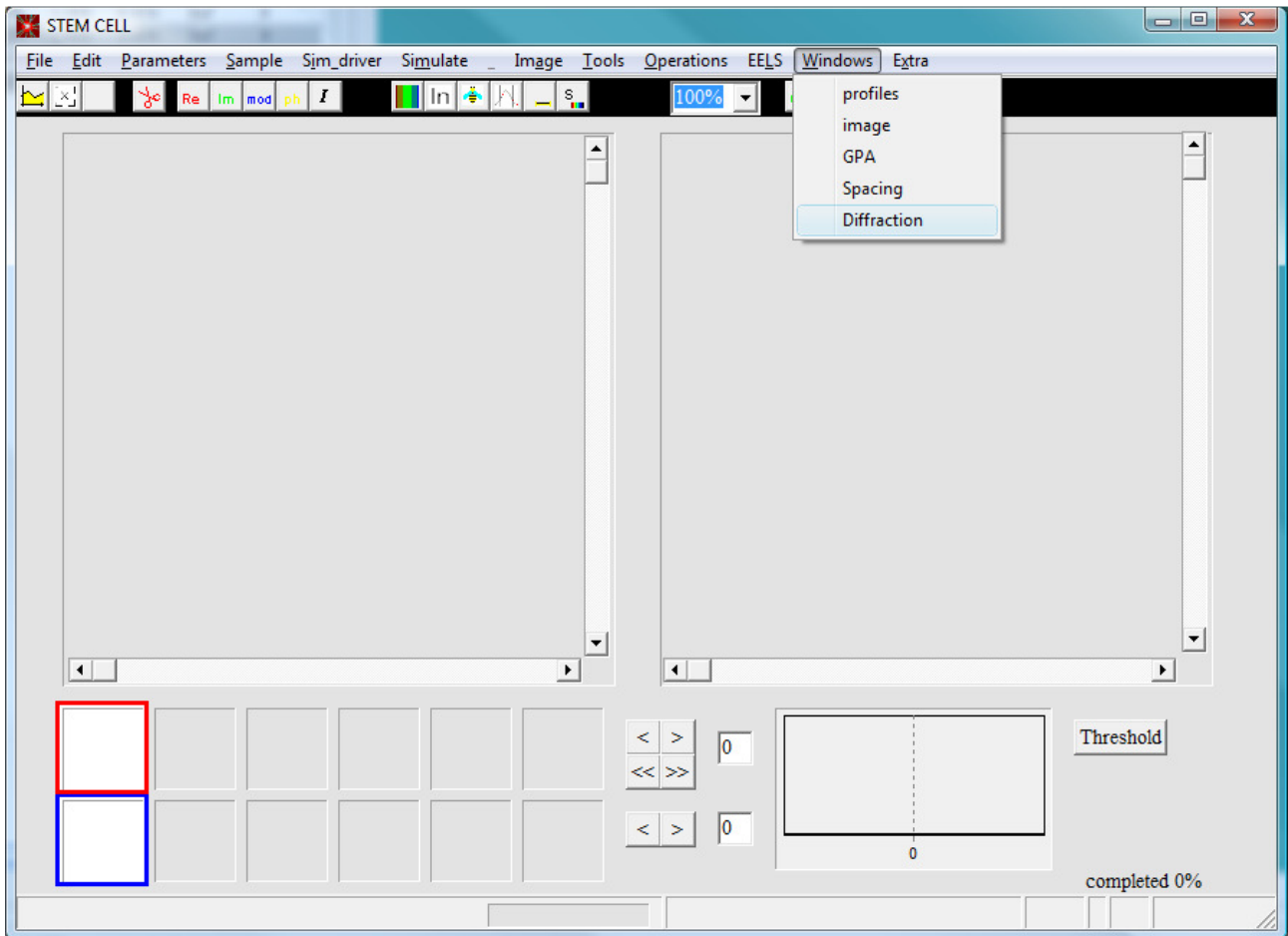
Show kinematically forbidden       Show extinction lengths

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-> diffraction



In this way a diffraction windows appears.

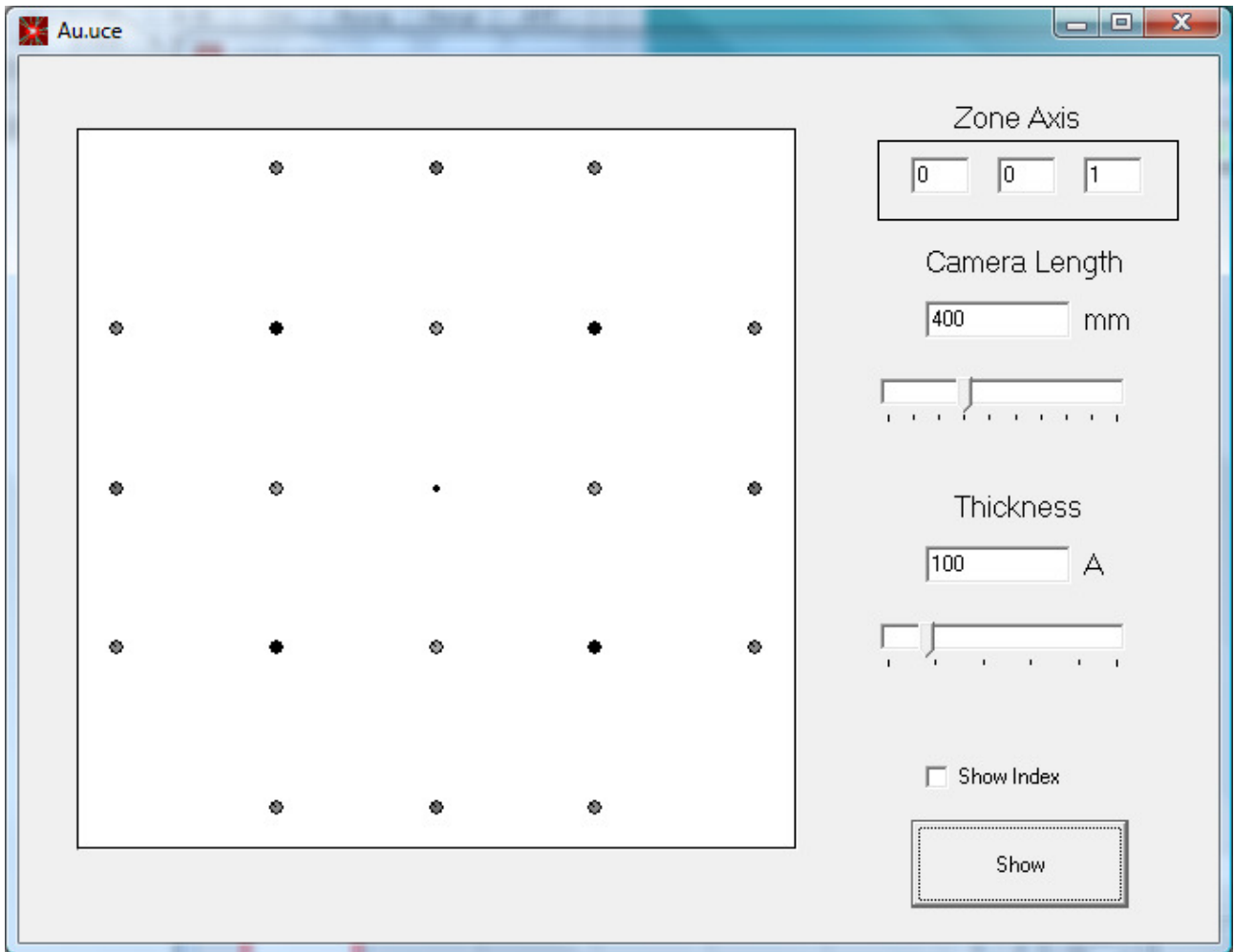
The most important number here below indicated by a rectangle can be set to define the zone axis to be visualized.

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.

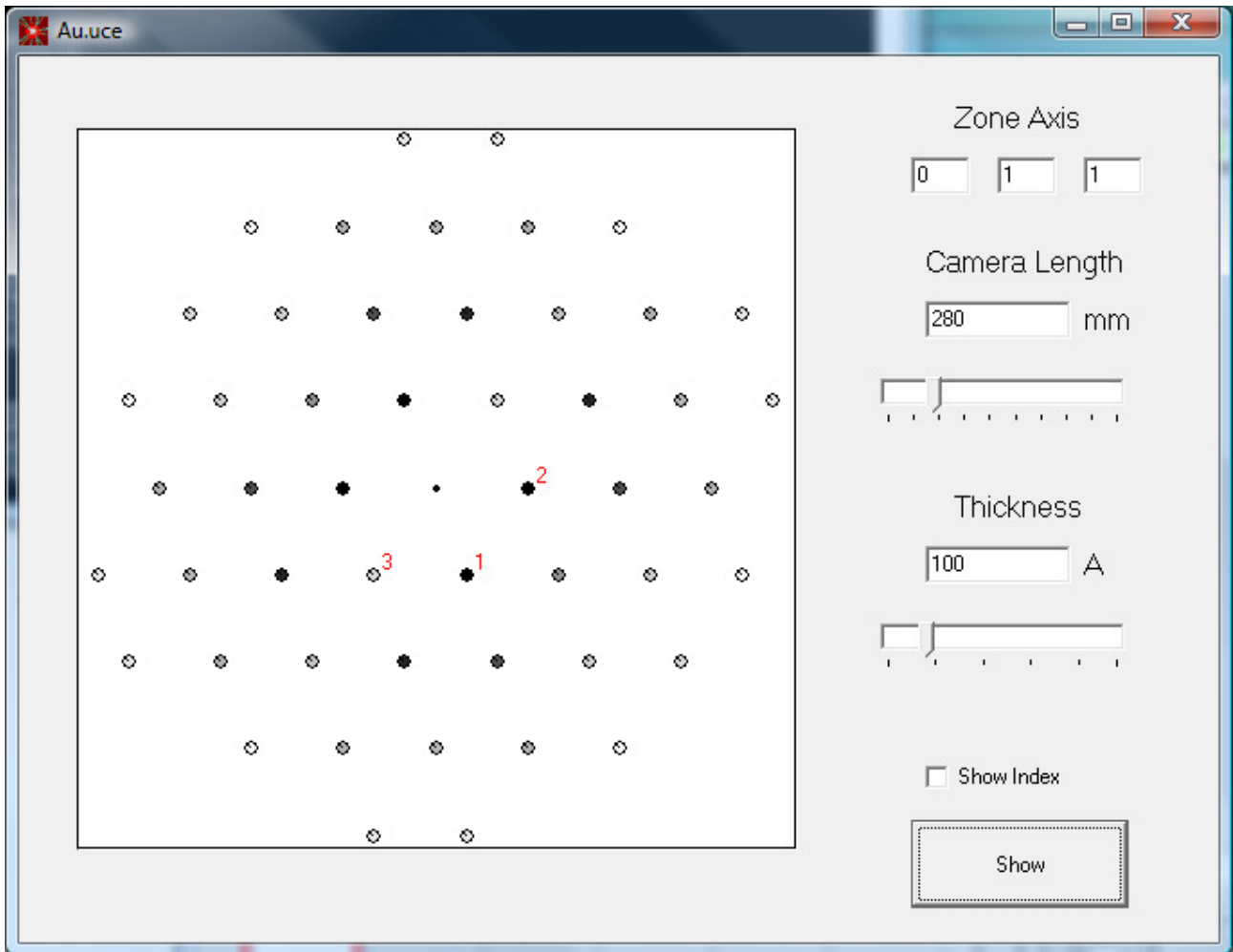
If you tick the “show index2 box and “show2 you can visualize the index of the reflections.





### 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.



```

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 (Å)   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 (Å)   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
  
```