SUPERCELL MANAGING (for version >2.3.1)

This document is meant as an introduction to the supercell mananging.

A few examples are shown here .

1) A core-shell nanoparticleof InGaAs/GaAs
2) A particle attached to a rod

Example 1

Unit cell generation

The starting point is the generation of the unit cell. For this example the cell can be generated from inside STEM_CELL using the part dedicated to semiconductor.

Sample->simple_gen

This open the special cell generator for semiconductor

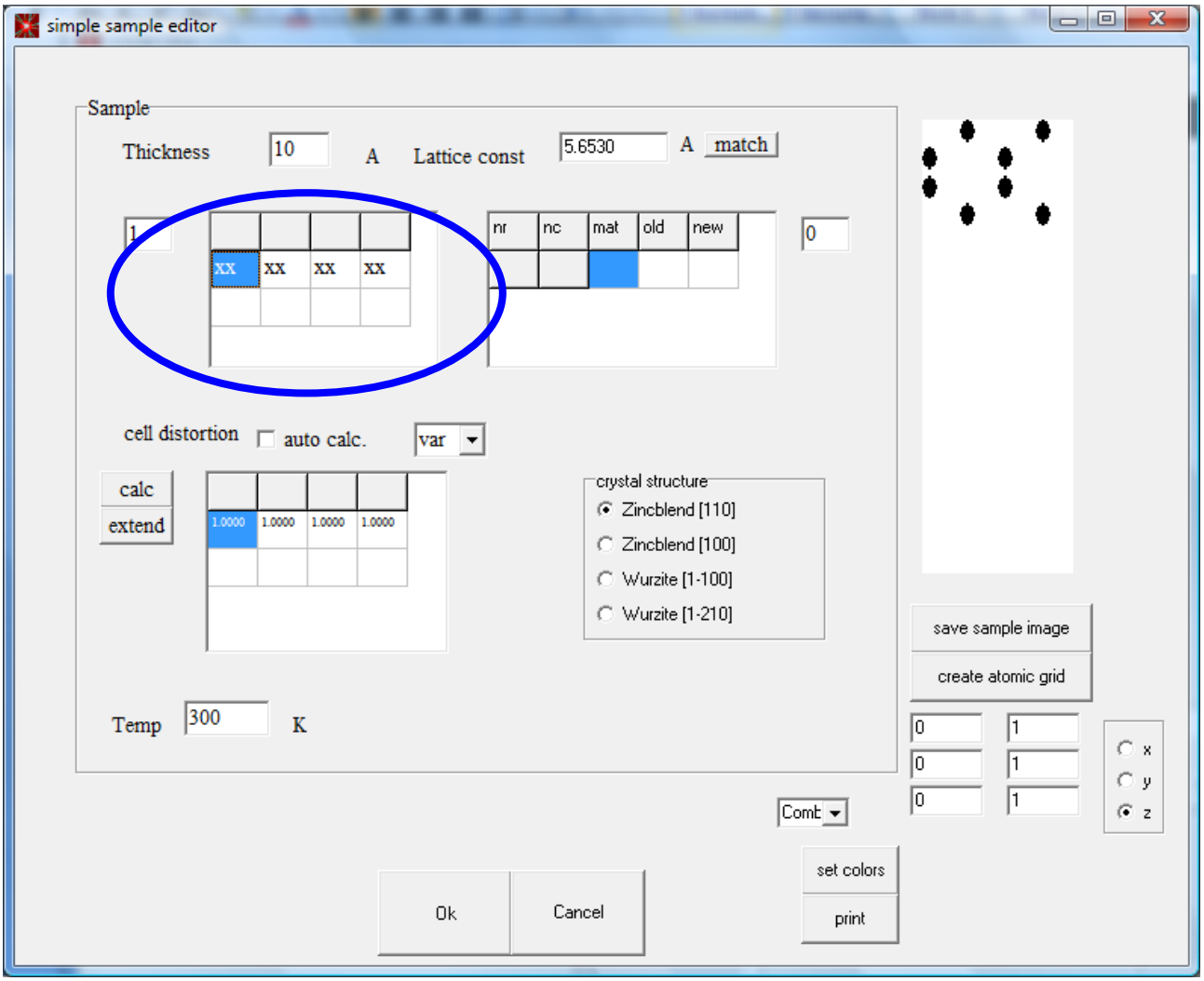


Fig 1

This module has many functions for semiconductor heterostructures but will be used here for the GaAs cell generator.

A list of supported material with a database of elastic properties is contained in the file *material_ext.txt.* In the database directory (selected during the installation).

As a first point the *crystal_structure* is selected by choosing between Zincblend and Wurtzite in 2 different axes.

We will select ZB [10 0]. Fig 1 indicates a box where atomic species should be inserted. The 4 position should be filled with a sequence *Ga As Ga As Ga As Ga As*

Trick: To simplify the insertion it is possible to write only the first Ga As and then use an automatic fill function.

Right click on the box and in the popup men press *Fill line*

Select now the match button , this sets the virtual substrate lattice parameter equal to that of the generated material in this case 5,653. If the lattice parameters is set to a different number *a* , the unit cell will be generated with *a* as lattice parameter.

If the match function gives 0 it means that you did not set the environmental variable TEMSIM.

~~Open a DOS shell and write~~

~~setx TEMSIM *<the directory you have chosen for the database installation>*~~

~~then restart stem_cell. This command has to be written only once since has permanent effect~~

With new installers theprocedure should completely automatic so at best download the ne installer from the web site.

You can now close the sample generation window by OK

The command Sample-> FS->MS2 creates the 3D model

Alternative method

If a JEMS or xyz GaAs unit cell is available it is possible to load it directly.

File->Open->Sample

OR

You can use the unit cell generator (see next example)

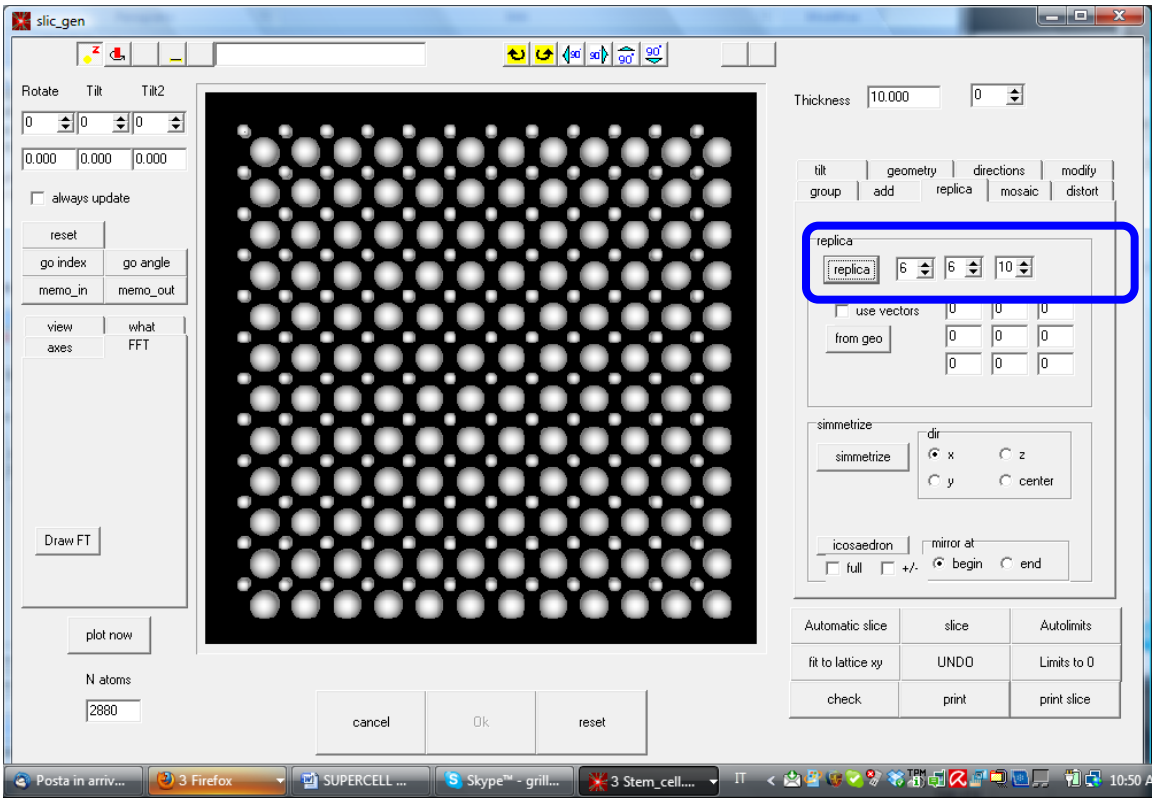
Supercell elaboration generalities

In this section the GaAs cell will be duplicated and a partial occupation will beaded in a selected region to form a core sell.

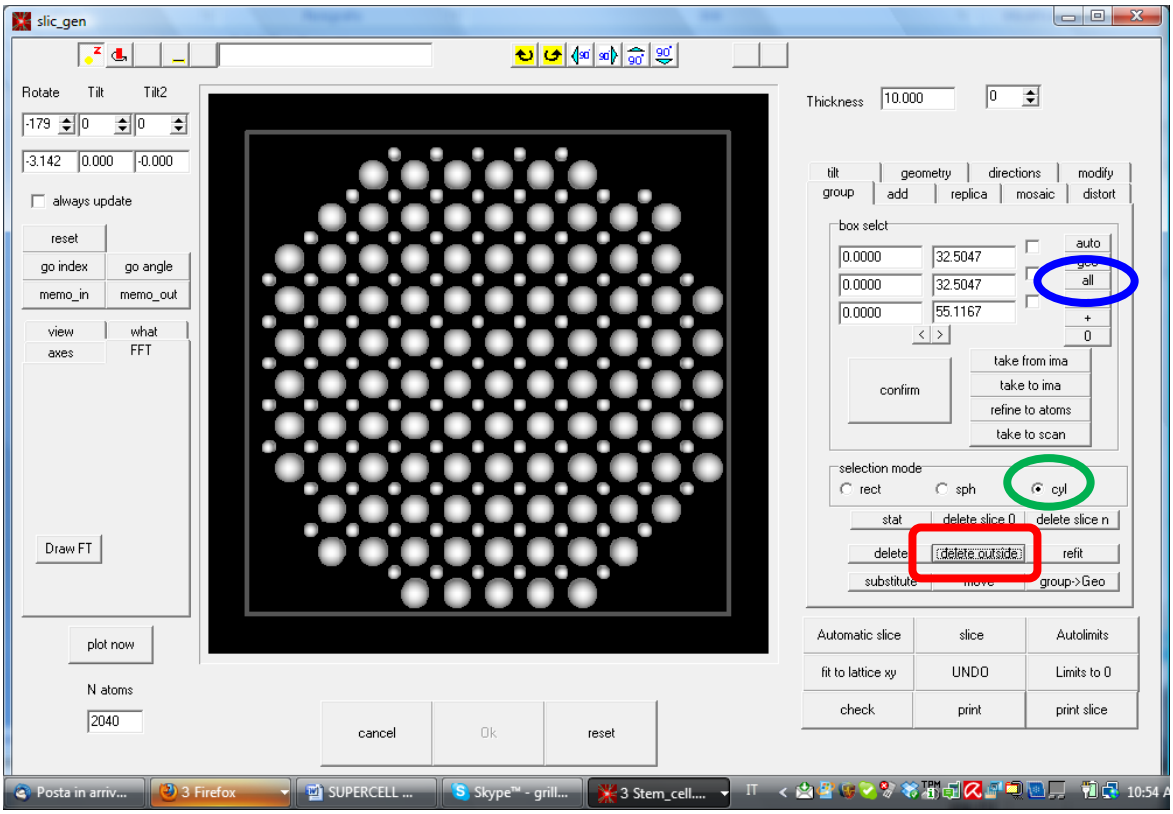
Press Sample->Slice_gen to open the slic_gen module

This module contains many information about the cell and many possible changes can be done. TO have a general overview of this module take a look at the appendix 1 (strongly advised).

We will now replicate the unit cell, go to *replica* tab, select 6,6,10

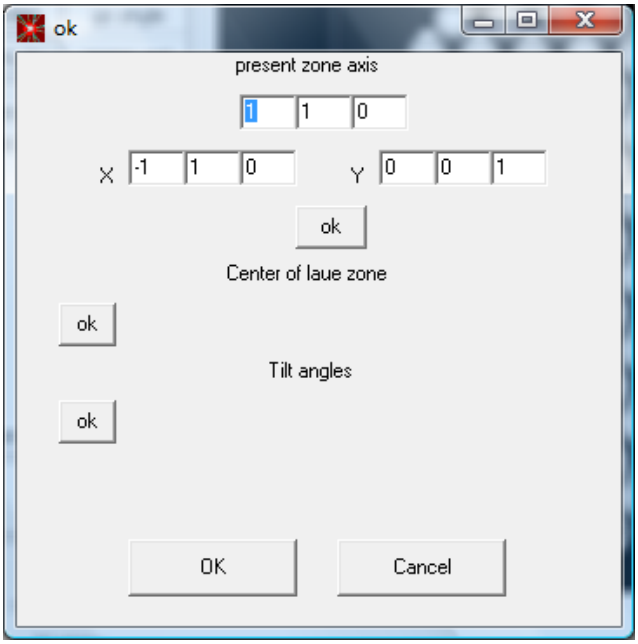


Now we will crop a cylindrical particle, Go to the group *tab* and select all.

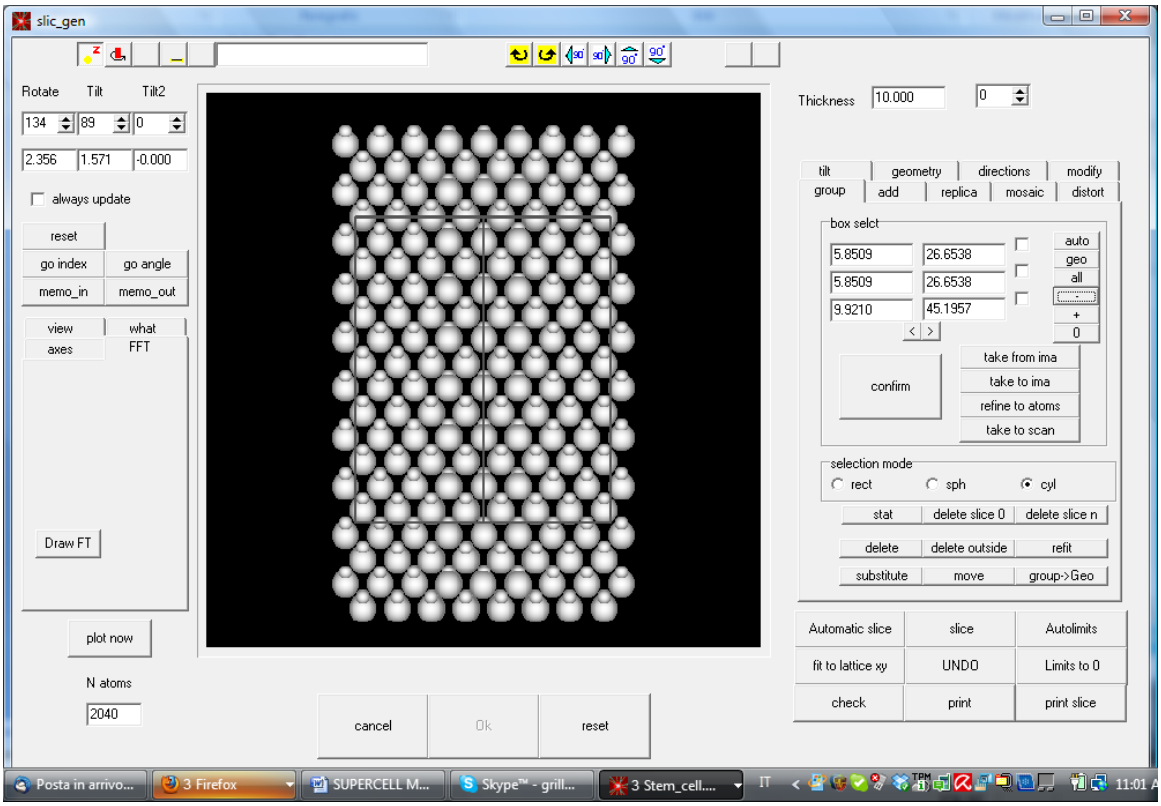


Then select *cylindrical* mode (green in the above picture) and press the *delete outside* button.

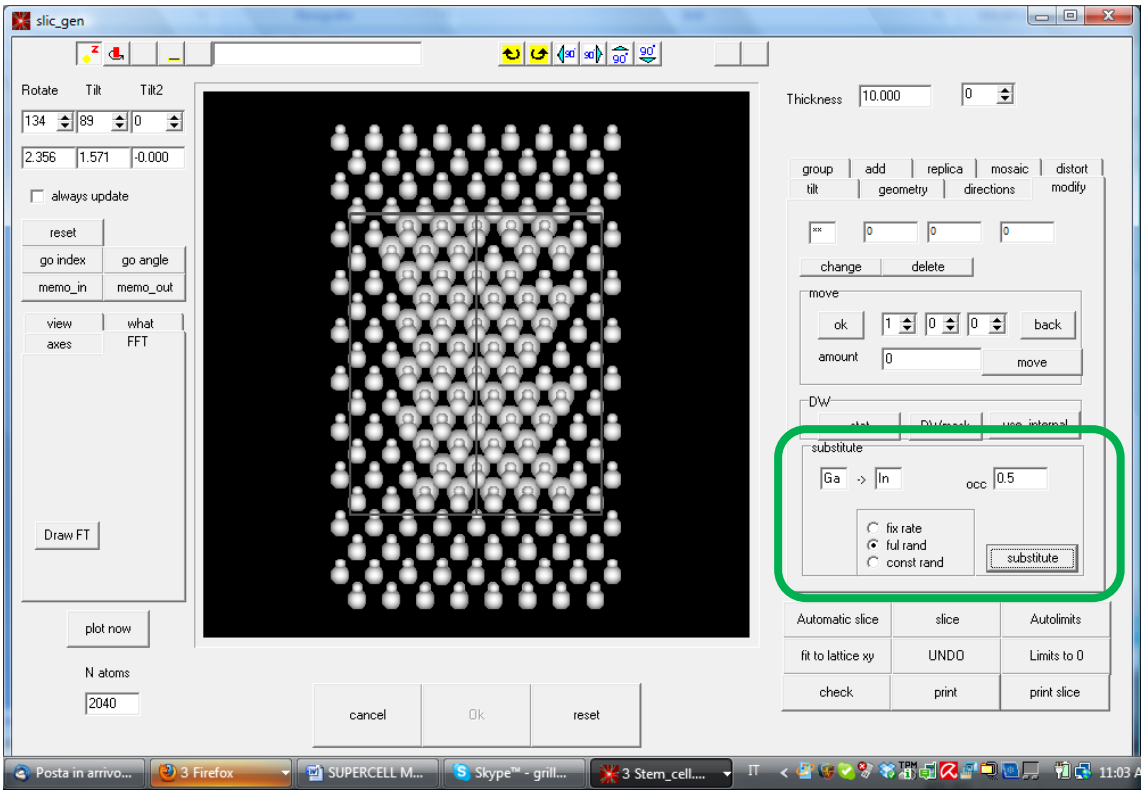
We cn take a look at the structure from side , press *go index.* And fill in the zone axis and the X as in the picture (pressing small ok Y will be updated)



In the group tab select the “-“ buton twice, this can be used to select the region where a core should be put.

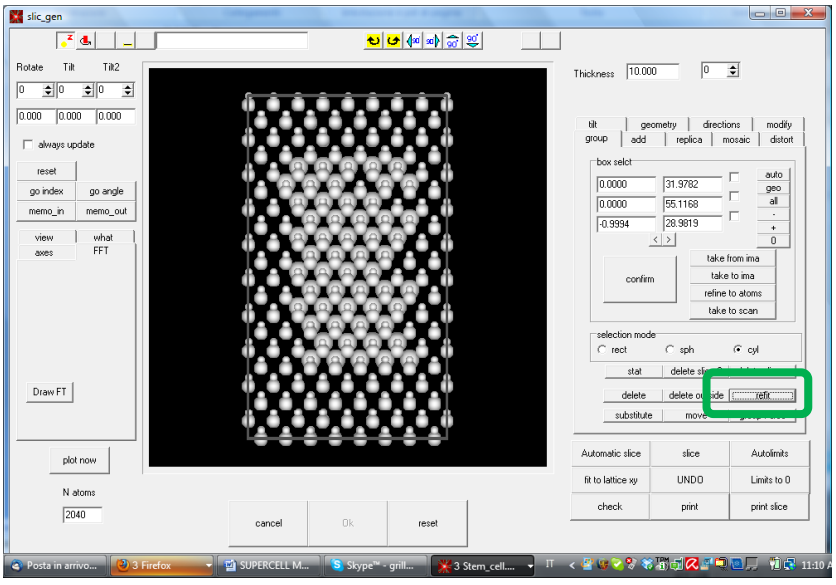


Now go to the *modify* tab , select Ga and In the partial substitution box (as in figure) and a partial occupation of 50%, then press substitute.



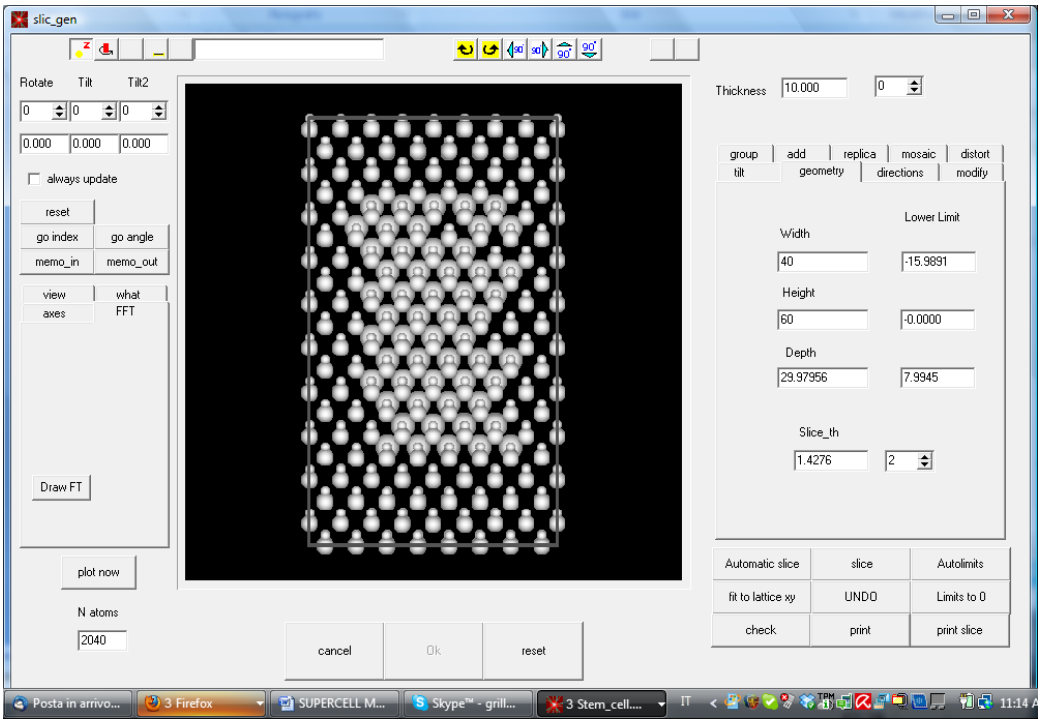
In the *direction* TAB select *actual cell rotation* and in the *group* tab select *refit* .

The actual cell rotation makes the current view as the slicing direction, the refit fits the grometry to the current size of the object in the new direction. Since this narrow geometry of the supercell may create problem with boundary conditions in the simulation it is advisable to select a larger geometry.



Go in the Geometry tab and select a larger cell then press *slice*.

If you want to visualize the new borders go to the *group* tab and select the *geo* button.



The structure is now ready for simulation.

It is advisable that you close the slic_gen module and save the structure

File->SaveSample

(select the krk extension)

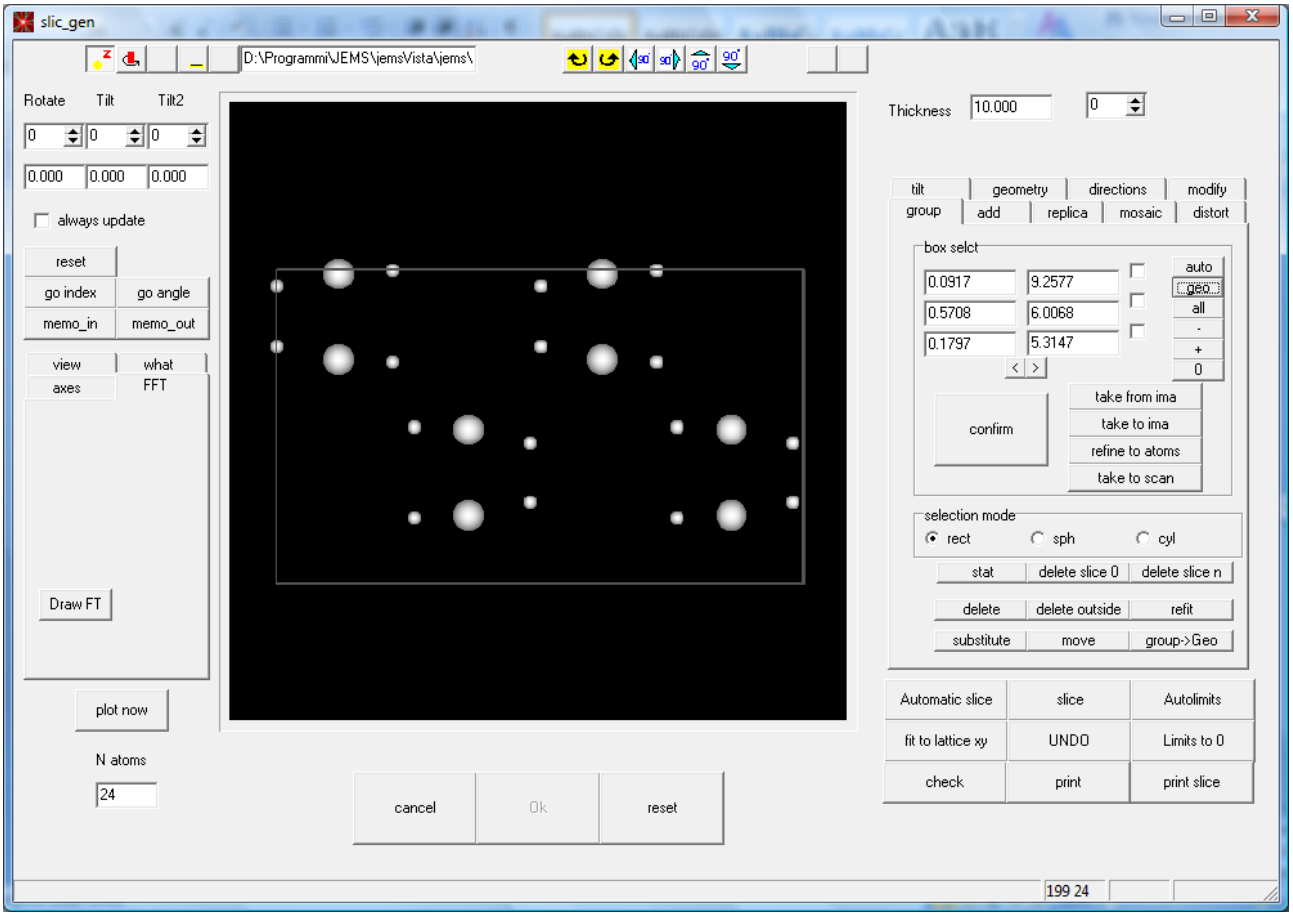
Example 2

For this supercell we will need a brookite (TiO_2)unitcell and a Fe3O4 unit cell. It is assumed that a JEMS cell is available. If this is not the case you can produce your own unit cell using the unit cell generator.

The creation of a unit cell is described in appendix 1. A support for CIF format will be also soon available.

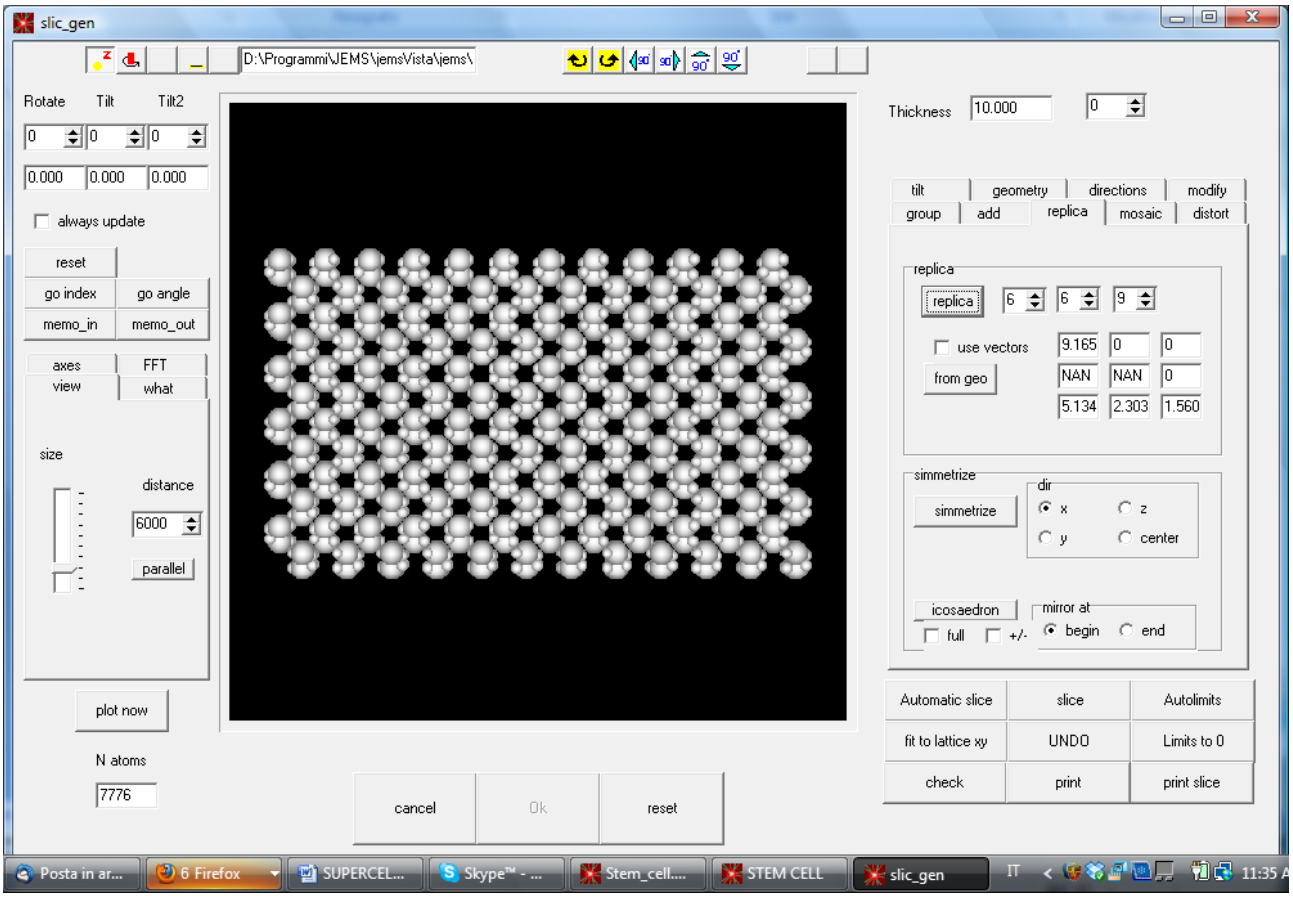
If you have the JEMS files Load the brookite file File-> Open Sample and select brookite.

Open slice gen



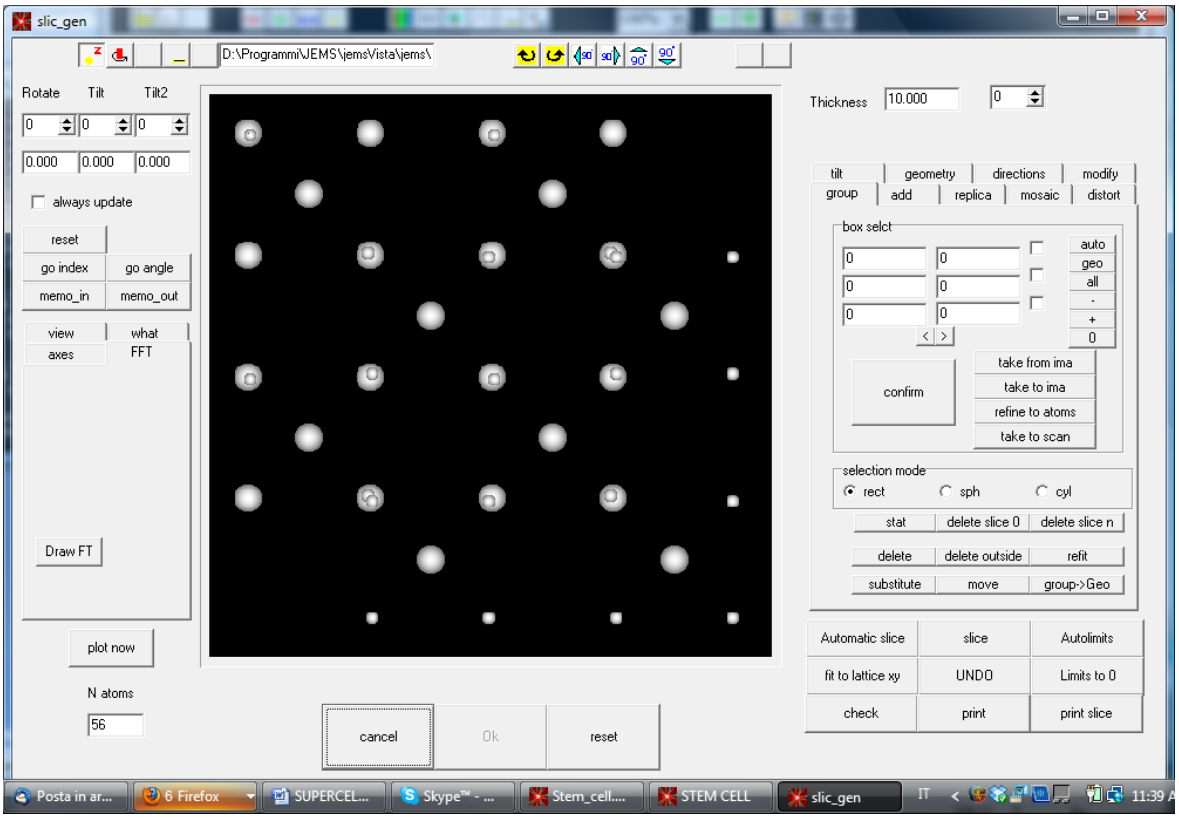
Replicate it by 6,6,9 times. For a better visualization of the cell go in the view tab on the left and sreduce it by at least 2 steps.

Now press *slice* and save the file in a krk format.



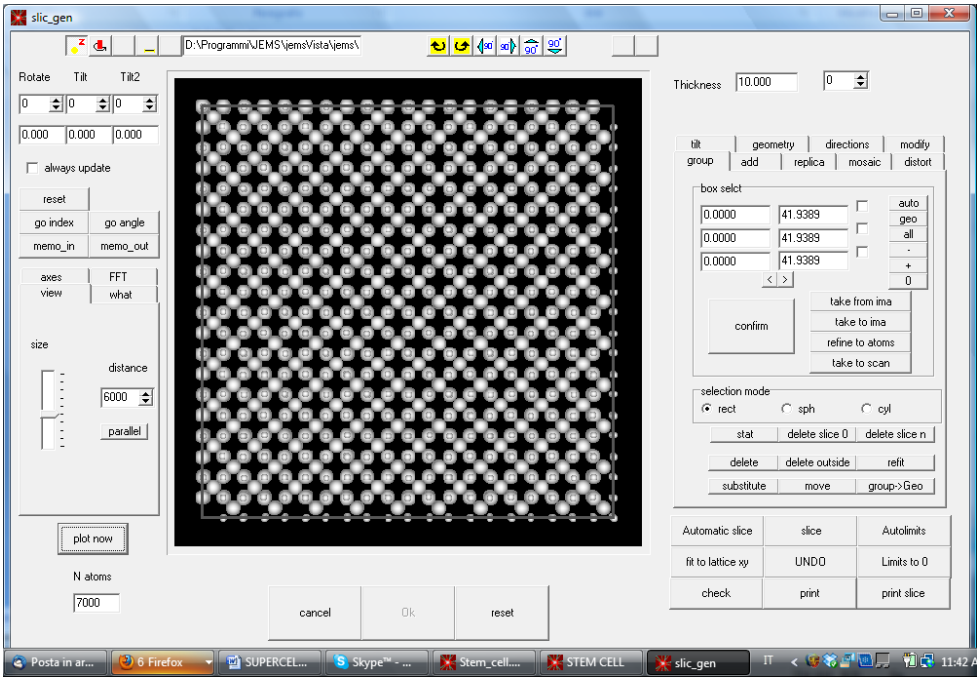
Second part: the Fe3O4 ball

Load the Fe3O4 unit cell as above. The unit cell should look as in the picture below. I use a cubic approximation of the Fe3O4 strcucture.

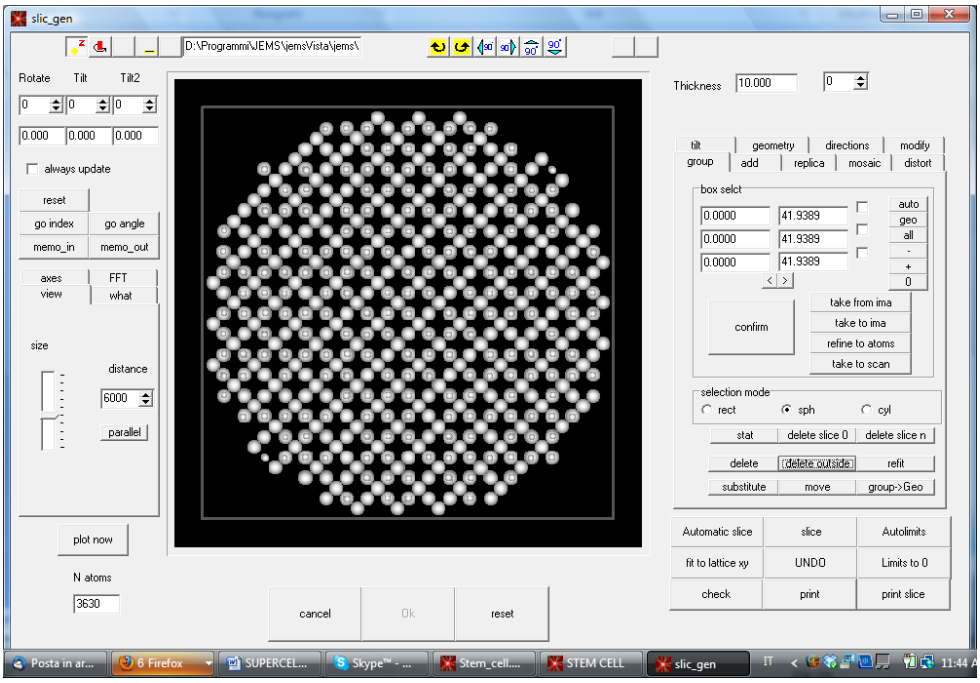


Replicate it five time (replica with 5,5,5). Then select it all by selecting tab *group* and then *all*.

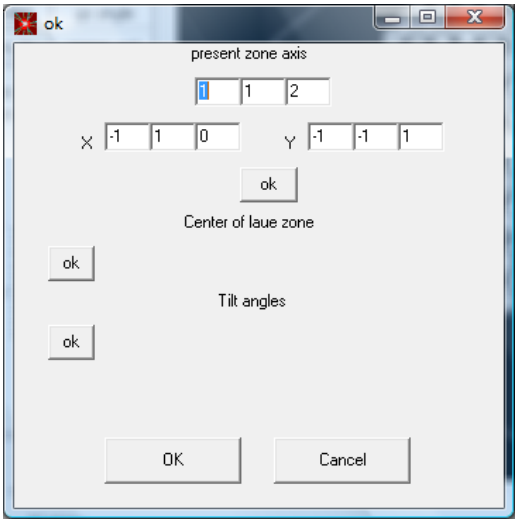
It is also advisable to reduce the atom size in the *view* tab on the left .



Select a sphere and delete outside



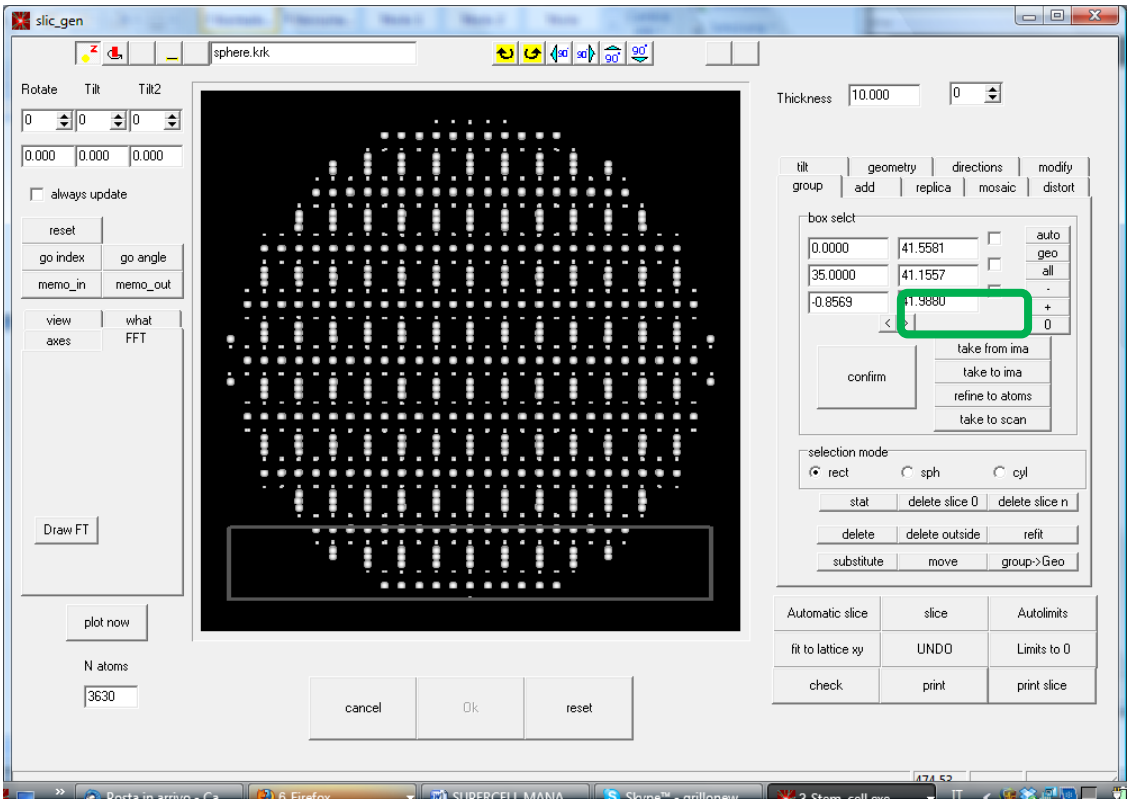
Change zone axis to the 112



And in the *direction* tab set *actual cell rotation.*In the *modify* tab set *refit.*

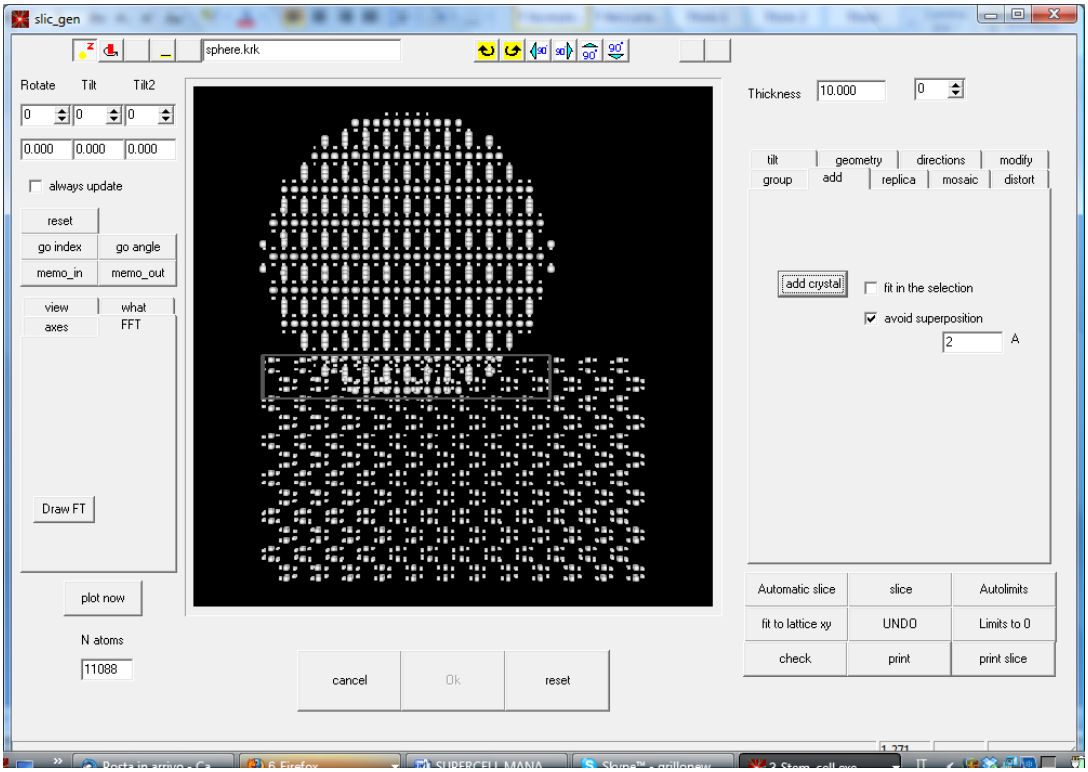
IN the *group* tab manually change the Y0 coordinate of the group from 0 to 35 as indicated in figure.

We are now about to add the rod: the position where it is goindg to be transate d depen on the first extreme of the group , that ‘s why we have modified it.



In the add tab select avoid superposition and then set 2in the box.

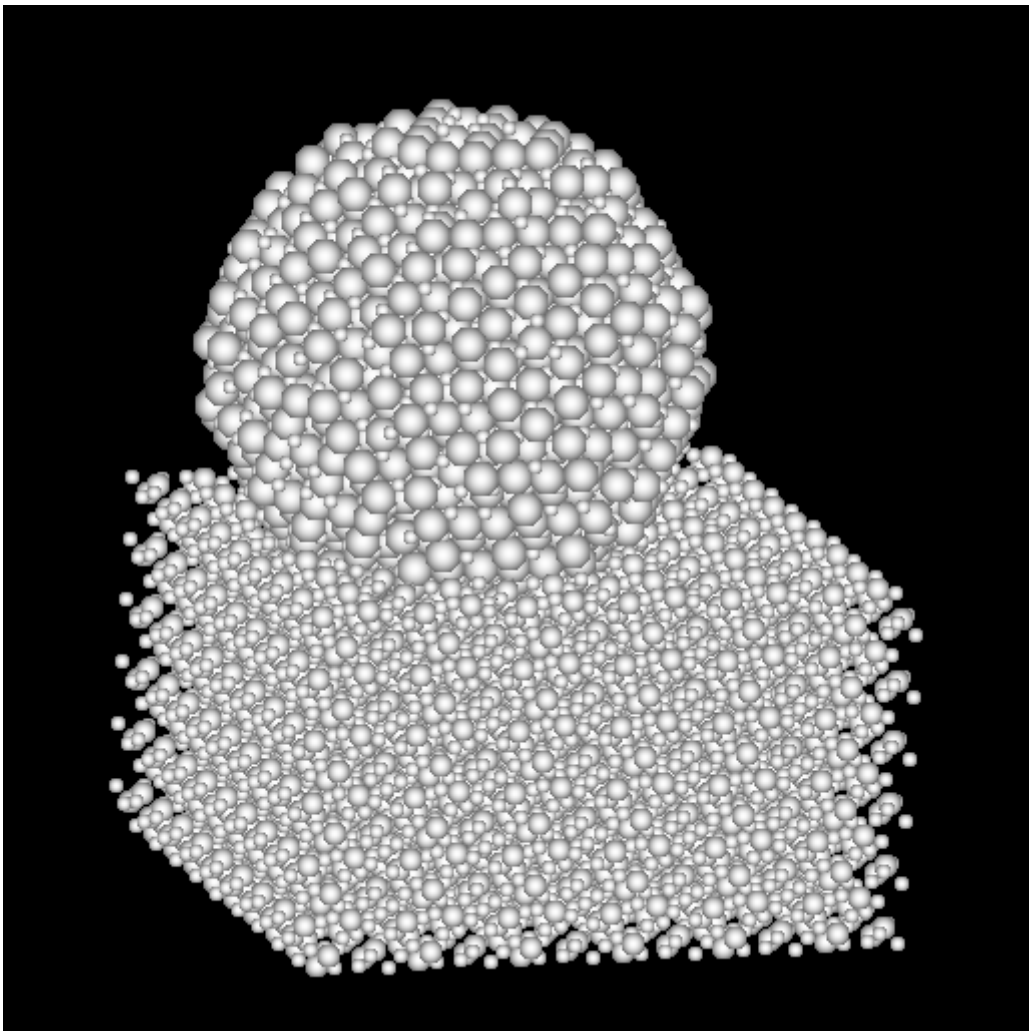
Then press *add-crystal* and load the previously saved TiO2 rod.



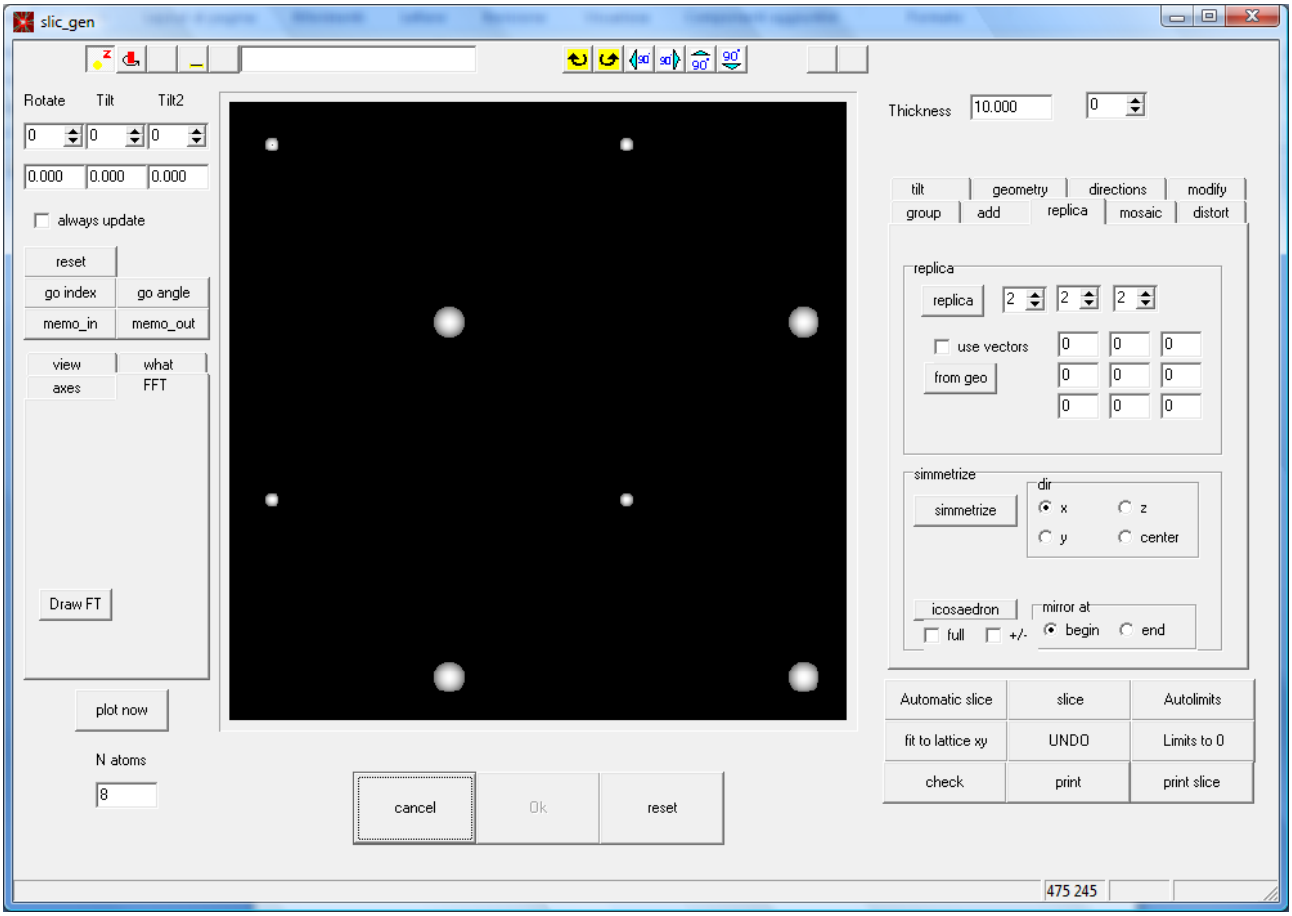
Press modify refit , adjust geometry and press the autoslice button.

We are now ready for simulation.

The structure here created has a complex 3D nature but TiO2 and Fe3O4 have no comenetation



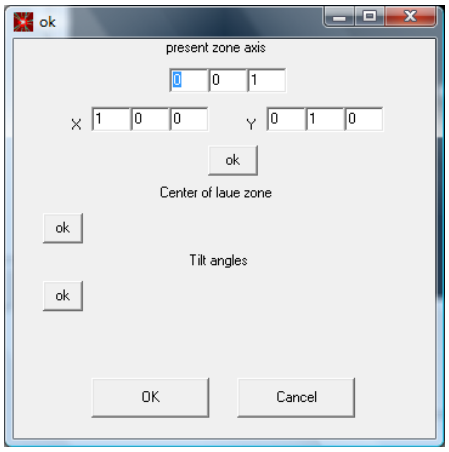
APPENDIX 1 :small manual of the SLIC_GEN Module



ROTATION

To better visualize the cell it is possible to rotate the visualization angle in 4 ways:

1) Change the Euler angle (rotate , tilt tilt2) explicitly in the left part. Then press *Go angle.* *Reset* brings all angles to 0 (original orientation), *mem_in* and *mem_out* can be used to store ad restore directions.
2) Press the  icon that sets the rotation mode : drag and drop the model to rotate it
3) The arrow  permit a perfect rotation of 90° from whatever angle, while in plan rotation by roughly 5°are obtained by pressing 
4) Press Go_index



This module permits to rotate cubic structures from one zone axis to another. Select the new zone axis and set the x direction. When pressing the small ok the Y is automatically adjusted.

Then press OK.

The support for non cubic structure is in progress.

It is important to understand that these rotations are only a change of visualization angle. If a real coordinate rotation is needed go in the *direction* tab and select *actual rotation.* This has the effect of make the rotation definitive : the present prospective becomes the basic slicing direction.

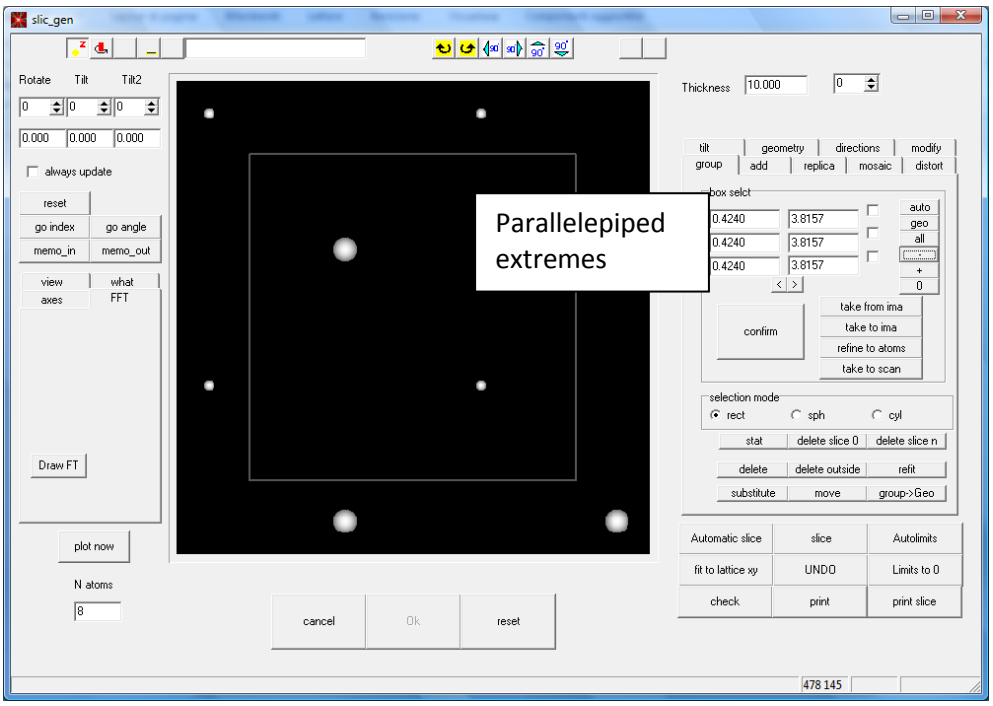
GEOMETRY

Selecting the *geometry* TAB on the right it is possible to visualize the supercell size and the initial point . The slice condition can be also selected.

More details in the end of this example

GROUP

Select the *group* tab to set a selection area useful for any kind of operation like cutting , moving or changing atom species. Group appear always as an parallelepiped, the extremes are the entries of the geometry box.



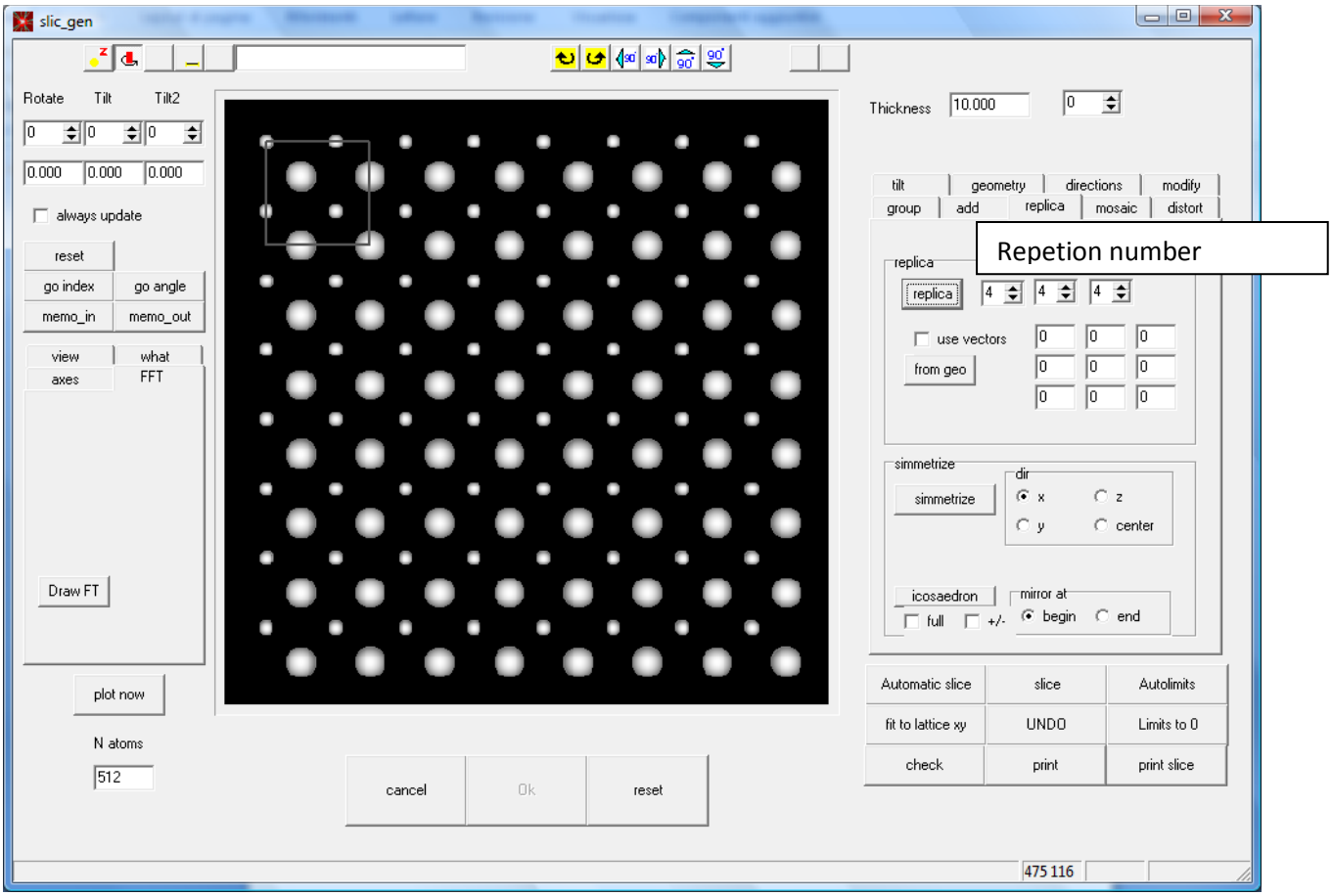
The group can be set in many ways

1) Pressing *all* a group is drawn stretching from the minimum atom the maximum value of the atomic coordinates.
2) Pressing *geo* the supercell geometry is transferred to the selection
3) Pressing – the selection is scaled down by about 20 toward the center
4) Pressing + the selection is scaled up by about 20 toward the center
5) Pressing *take from image* The selection is taked from the currently selected image in the main module.
6) The extremes of the parallelepiped can be also directly selected by changing the numerical value (then press confirm)

Even if graphically the selection appears as a parallelepiped it is possible to also select a sphere or a cylinder. In the latter case the axis is always along z

REPLICA

On the right panel select the *replica* tab.



The replica of the unit cell can be performed either in the coordinate direction (with spepc equal to the present cell size) or along 3 arbitrary translation vectors. For cells loaded from JEMS the translation vectors are automatically filled in. Select use vector for this second option (translation vectors should be written in the rows).

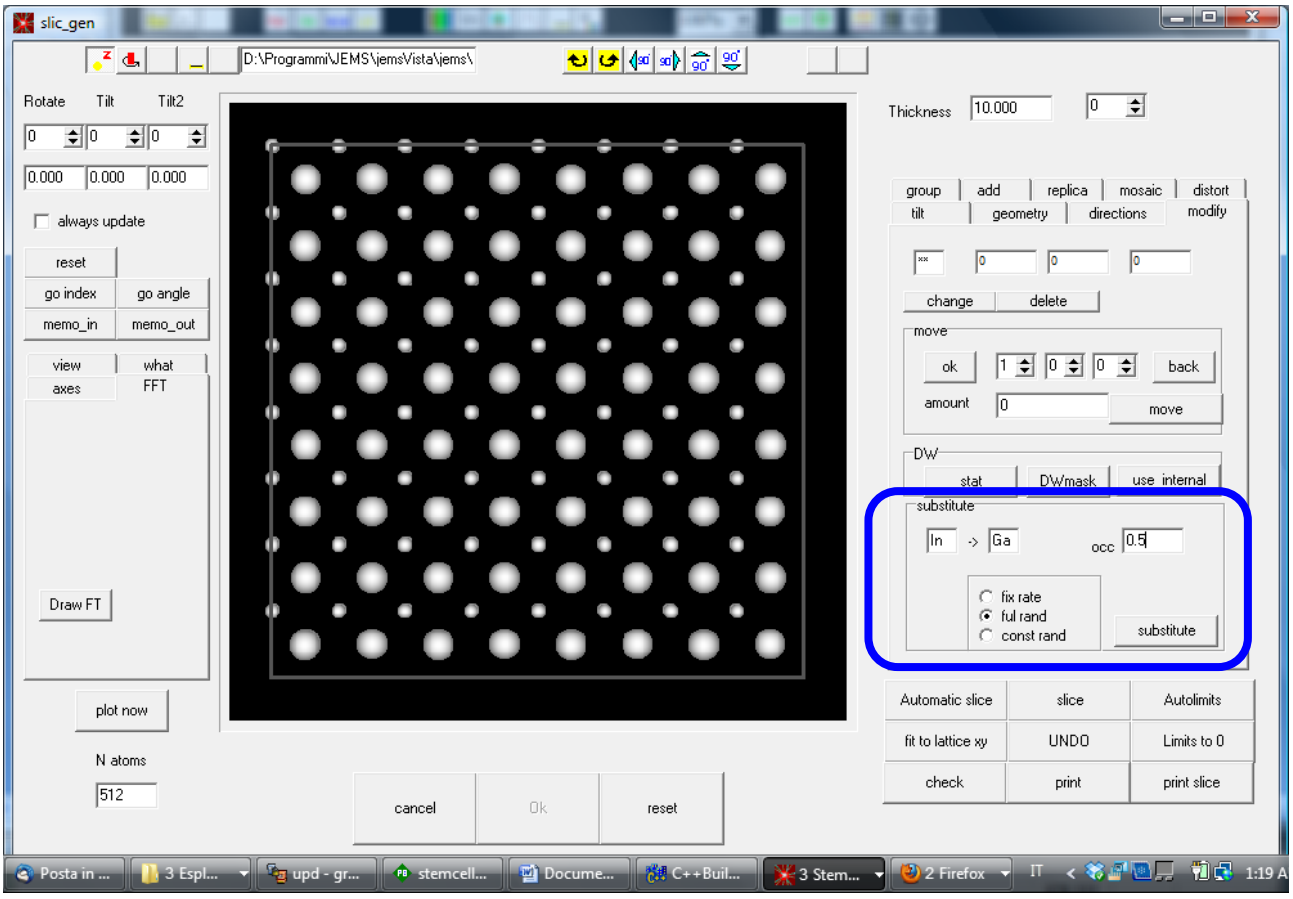
Select manually the repetition number in every direction.

NOTE The normal replica can be iterated many times but the replica with translation vector can be done only once.

DELETE OR CHANGE ATOMS

The atoms can be deleted selecting the appropriate group and its shape (parallelepiped, sphere or cylinder). In the *group* tab then press the *delete* to remove atom inside the selection and *delete outside* to remove the external atoms.

If the atoms need to be substituted select the group as above then select the *modify* ab



In the selected box it is possible to specify which atoms are substituted and with what , partial occupation needs also to be set. The kind of filling for the partial occupation can be also specified: *fully random* means that atomic places are randomly filled, *fixed rate* means that the places are filled according to a recurrence rule dictated by the partial occupation *const rand* means that the position are occupied with the contain of the total number of atom of each kind to be exactly correspondent partial occupancy.

ADD CRYSTAL

The add crystal tab can be used to load another model and add its atom to the present model.

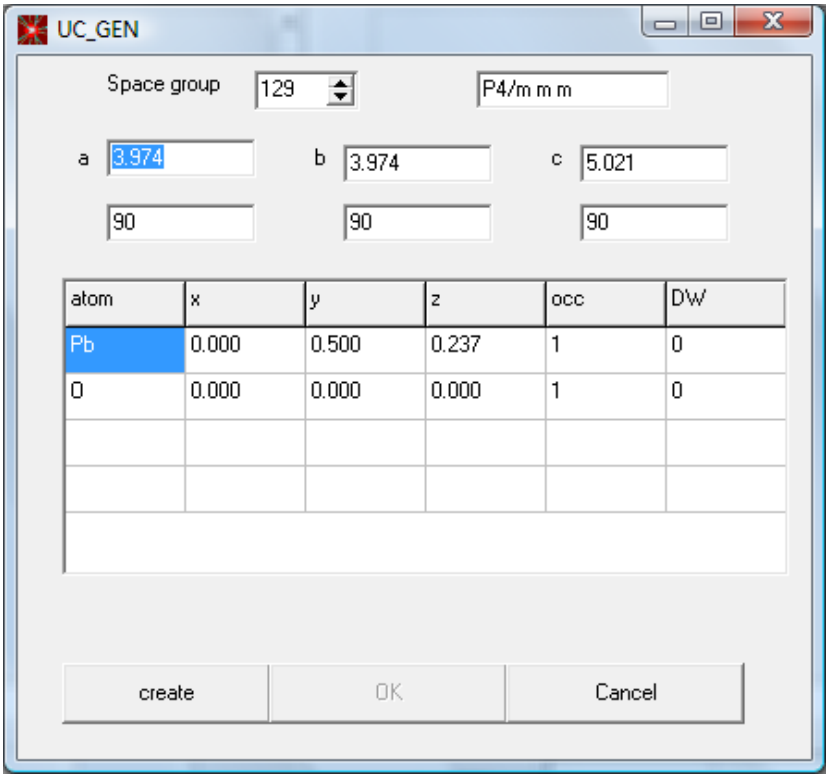
The atoms of the new files are translated by an about selected by the first extreme of the group box.

Setting *avoid superposition* permits to remove atoms that superimpose with a specified distance to the old cell atoms. Setting *fit in the selection* limits the added atoms to within the group second extreme.

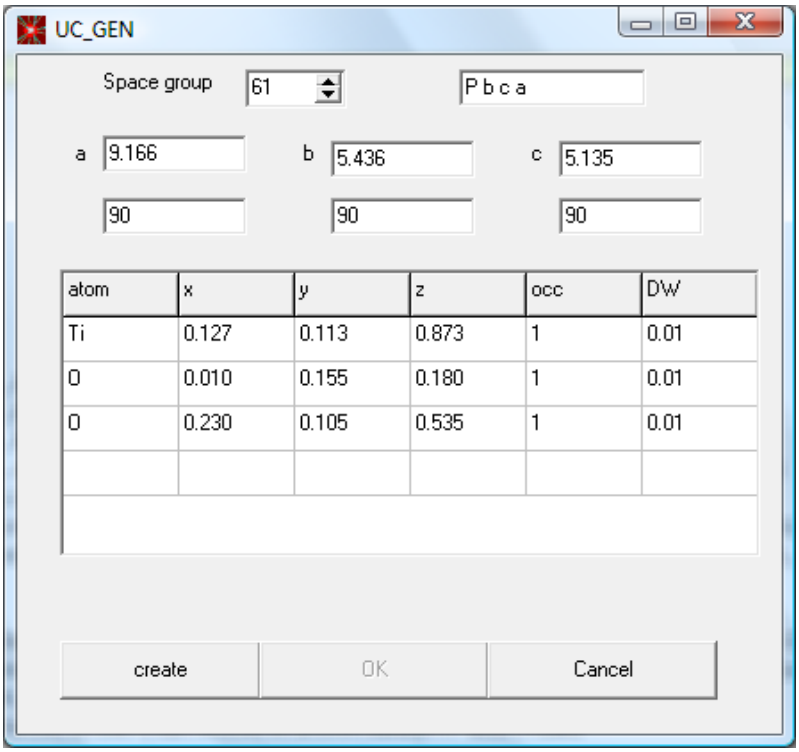
Appendix 1

To create a unit cell use the module *UC_GEN* that can be opened by

Sample->Unit_cell_gen



The screen should appears as in the picture. An example structure is already present , change group number , lattice parameters , angles and insert the base coordinates.



For example for the Brookite the module should be filled as in figure.

Press *create* and *OK* . It should be possible to visualize structure in the *slice_gen* module and operate the required manipulation.