Simulations with STEM_cell

The program can run simulations based on the well known kirkalnd routines [1] and with my version of these routines for (S)TEM simulation [2]. Sources of my small modification of these graphical routines are available upon request as required by GPL licensing.

The advantage is that everything is made graphically and that supercell manipulation can be performed.

Preliminary SETTINGS

With version > 2.3.1.3 no preliminary set are necessary

INPUT CELLS

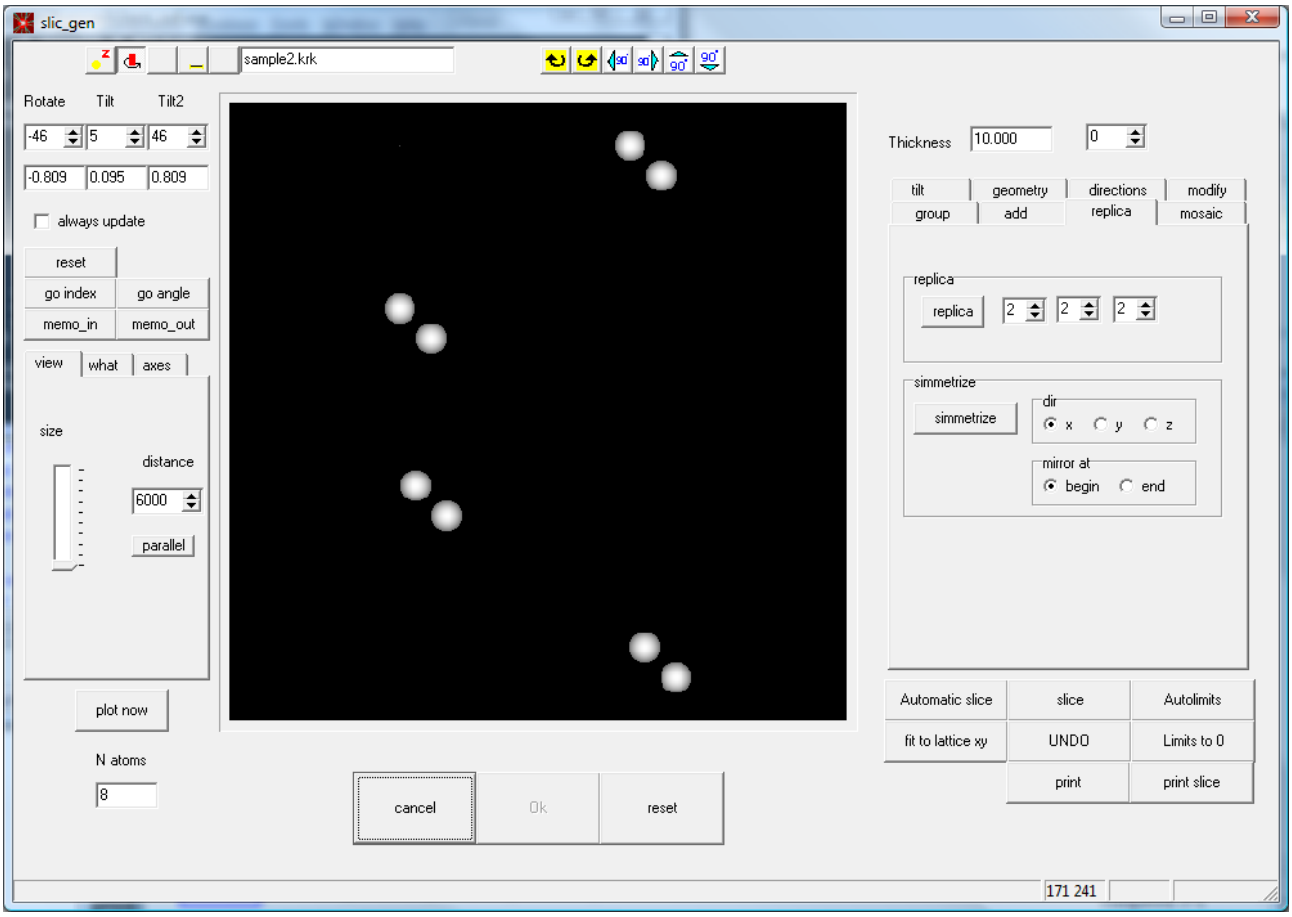
STEM CELL does not allow the creation of cells from scratch if not for a few particular cases related to semiconductors (spherelite and wurtzite structures).

For these cases it is possible to create FLAT SAMPLES …. More details on this are given in the appendix.

For all other kind of samples it is possible to import structures created by other programs (Mac Tempas, JEMS) or in the basic .xyz format. The special xyz format introduced by Kirkland for his simulation are given in this context the extension .krk and can be opened by STEM_CELL. To open the cells use FILE->Open sample. The file will be opened according to its extension.

CELL MANIPULATION

To open and manipulate the cells open Sample->slice_gen. Not ethat this mask is available only when you have already opened a cell file.



Screen shot of the cell manipulation mask

The general philosophy is that the command on the left (an the button on top) affect the visualization of the cell while the command on the right do substantial changes on the cell and its slicing.

Three euler angles rotations are possible by directly setting the numerical values and pressing “go to angle”.

The five top-left button set the mouse use… if the red (second) button is set it is possible to drag and drop to obtain the rotation of the cell.

Moreover if the cell has been imported in the [1,0,0] zone axis and it is based on a cubic unit cell, it is possible to directly rotate to a new zone axis (go index).

The command on the right permit to replicate, cut and add crystal pieces or to substitute atoms. A single UNDO is available for each step. Memory failure can occasionally occur so I recommend to save you cell from time to time.

To perform the most important modification it is useful to set a ROI or selection BOX …this can be done by going in the group tab and selecting the xyz limits of the box. They can be set automatically to the geometry limits, to the minimum box containing all atoms or to 0. It is also possible to pick a box from the 2D selection box in the foremost image if this is in the correct scale.

The most important function of this program is to optimize the slicing of your unit cell. You can do this by setting manually the slice thickness (in the “geometry” tab) or simply by pressing Automatic slice. Since also the lateral boundary conditions are important a periodic fit of the limit of the cell can be obtained by pressing “fit to lattice xy” (this is still under development so make sure that cell geometry is fitted upon your cell before using this function).

Alternatively you can set the geometrical limits to the minimum size containg all atoms. This is not advisable for simulations but can be useful for further elaborations

More on the specific command can be required writing

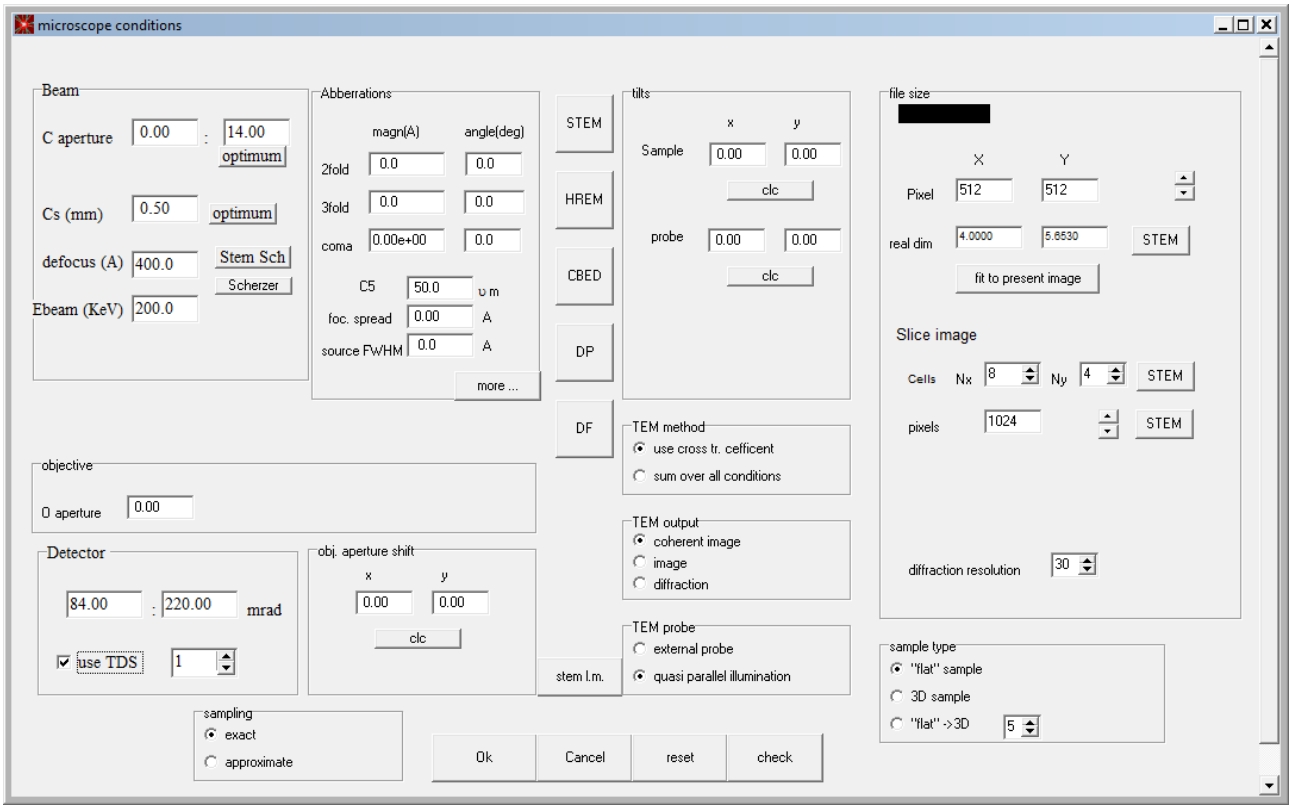
vincenzo.grillo@unimore.it

SIMULATION

Once the cell is ready you can start a real simulation … possible simulated techniques are TEM , diffraction, STEM , CBED. The settings for each techniques are different.

TEM SIMULATION

Open the Parameters->beam/det mask.



Main parameters window.

The first important thing to do is to specify that you want simulate a 3D cell… (“flat” are the special cells mainly for semiconductors see appendix).

The general philosophy (with few exceptions) of this mask is that the left parameters are the physical parameters while the right ones are simulation setting and details …

In order to facilitate the set of appropriate parameters a HREM button has been prepared that loads a reasonable preset of values for your TEM imaging and checks for the most appropriate setting for the sampling.

If you are done with the choice of the physical parameters try retyping the button HREM to check the sampling and if the physical values you have set have a meaning (e.g. if the spread of focus is less the 1 A it will be set to 70 A).

After this press ok.

You can now go to Sim-driver-> Tem-> autoslice that will run the simulation in the non graphic window.

The final results will be opened automatically.

NOTES on Kirkland's routines

Depending on the simulation scheme you are using the simulation works in a slightly different ways.

If transmission cross coefficient (TCC) approach is used the autoslice program will produce the file **wav.tif** containing the exit wave function. This will serve as a input for the image program that will produce the final image on screen **TEM.tif.** Both operations are automatically performed by STEM_CELL an dthe final results is automatically opened.

If the more pedant approach is used the autoslice program will directly produce the **TEM.tif** file opened automatically by STEM PRO.

Note also that at the moment the programs do not contain a loop over frozen phonon configurations so if you want to use this algorithm you have to perform many simulation and average them (this can be done with some trick in STEM CELL). I will produce a custom version of autoslice curing this problem some time.

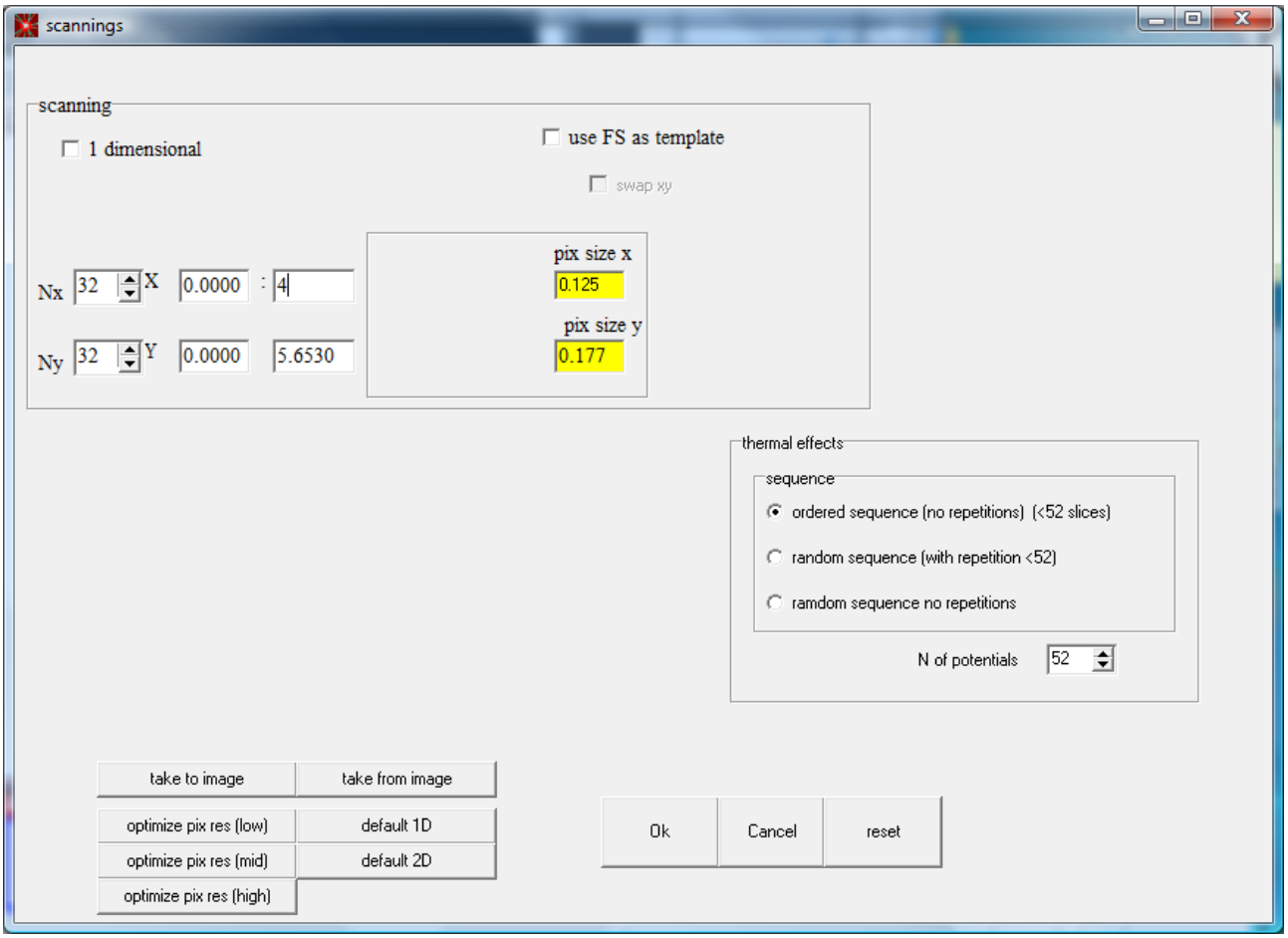
STEM

Stem simulations are more complicated but the main step is similar to what seen above.

- Open the Parameters->beam/det mask.
- specify that you want simulate a 3D cell (see above)
- Set the physical parameters
- Press STEM.
- Press Ok

Now go in the Scanning window

Open the Parameters->scanning



This windows permits to set the scanning size and the number of pixels in the scanned image. In the yellow boxes the corresponding spatial setting is indicated. Some presets for different resolutions can be used to set the number of pixels once the real space limits of the scanning zone have been set. These can be loaded from and to the foremost image.

The work to implement “default 2D” and “default 1D” are under progress.

Finally it is possible to set a few parameters by pressing Parameters->loop that permit to perform loops on a selected parameter(still under progress for autostem) or to obtain the intermediate data for different thickness and/or detector angles.

More details can be obtained by email at vincenzo.grillo@unimore.it

The execution of the actual simulation is performed by pressing Sim_driver->STEM->autostem

The results **detected.tif** is automatically opened (version >2.2.4) but if you produced extra files for different detectors or intermediate thickness these should be manually opened.

The driving of autostem is still under test so bugs are certainly possible.

Instead of the autostem program in the kikrland routine there exist also a few executable made by me on the basis of Kirkland routines . Many of which use parallel computing but these are available only upon collaboration.

LINEAR IMAGE SIMULATIONS

For a first check and to set the scanning parameters you can simulate STEM images by simple linear convolution with the probe. This can be performed by Simulate->linear image approximation.

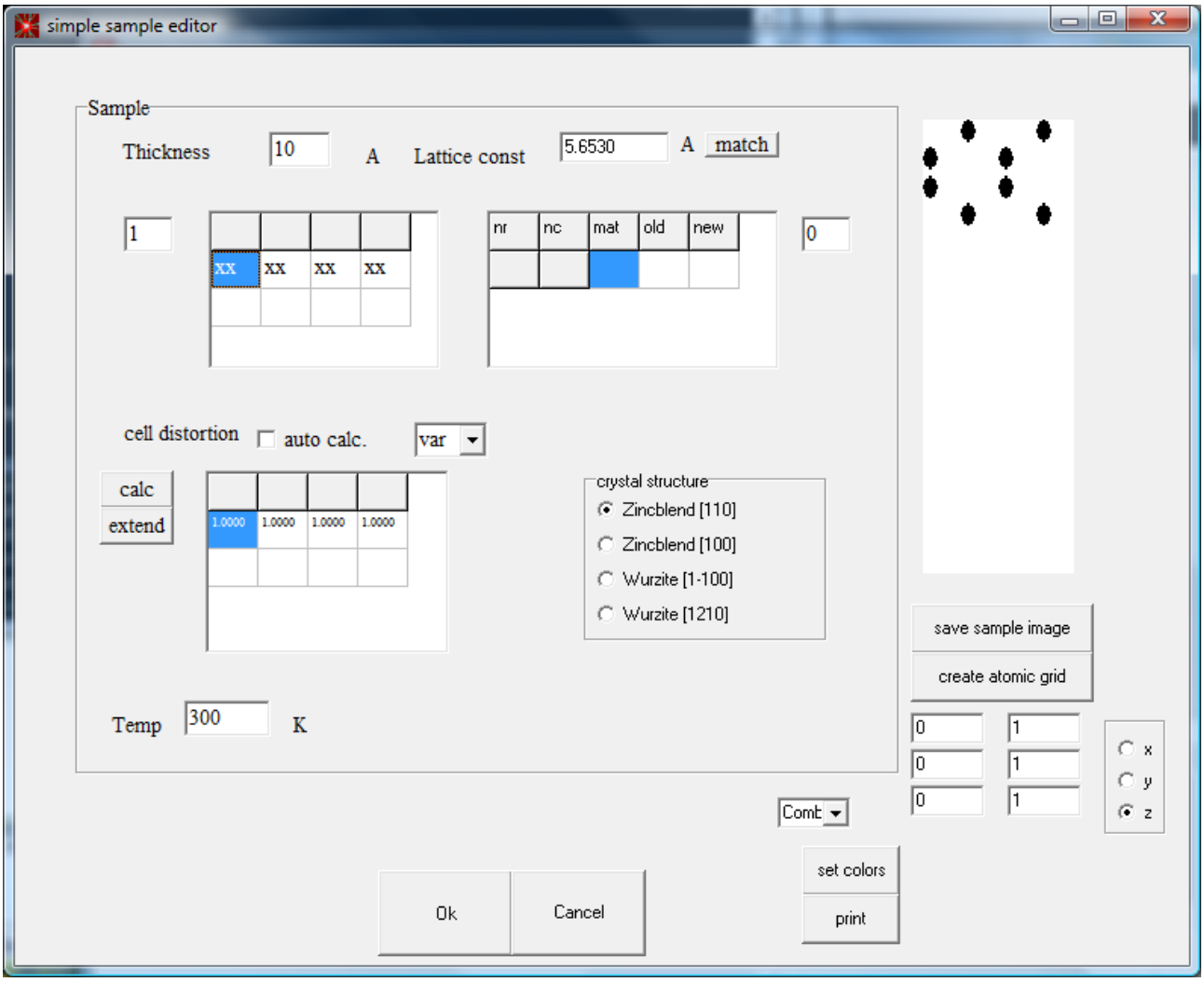
The object function is given in this case by the potentials of the sampole you have in memory . If you need the potential to be (more realistic but slower) squared you can go at Extra->options

In the simulation tab check square potential in linear image.

APPENDIX1: Flat samples

It is possible to quickly construct spherelite or wurtzite structure in a few zone axis … this makes sense only for semiconductors.

It is possible to do this by performing by pressing Sample->simple gen



The first box can be fille with the name of the atoms. The second permits to control partial occupations. The third controls the tetragonal distortion.

So first fill the first line for example typing GaAsGaAs then point the mouse on the point where you want partial substitution and right click. In the menu select “partial occupation”. This will drive you directly on the second frame where you can select the new element (say In) and the occupancy of the new element (the new will be automatically sett as 1- old).

Finally press calc to calculate the elongation of the cell in the z ”growth” direction. Notice that this calculation depends on the substrate lattice parameters (box in the top left).

When you are finished press Ok , Notice that a check is performed on wether your partial occupation is meaning full considering your specimen thickness (namely the integer number of atoms). If you do not want to care about this just press ok.

If you need to use in detail this function email at vincenzo.grillo@unimore.it

Notice that you can transform a flat sample in a normal 3D sample just by selecting Sample->Fs-Ms2.

[1] http://people.ccmr.cornell.edu/~kirkland/

[2] http://tem-s3.nano.cnr.it/software