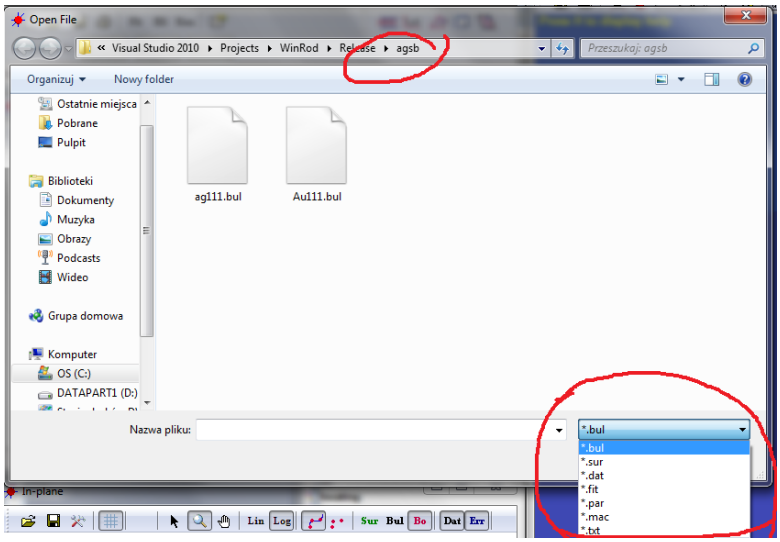
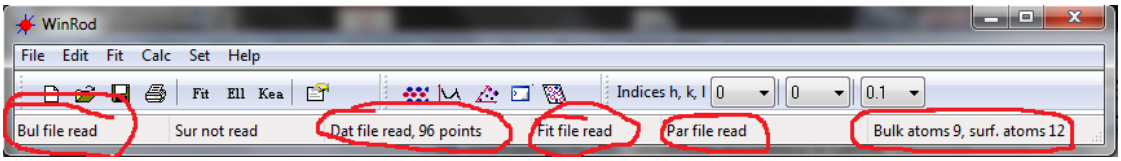
Fast start

In this short description, all import phases of surface x-ray data modeling with WinRod are presented. This program was created to make the surface X-ray data analysis more simple and faster. Most of the ideas are directly taken form ROD program originally written by Prof. Elias Vlieg. WinRod uses modified calculation engine from ROD.

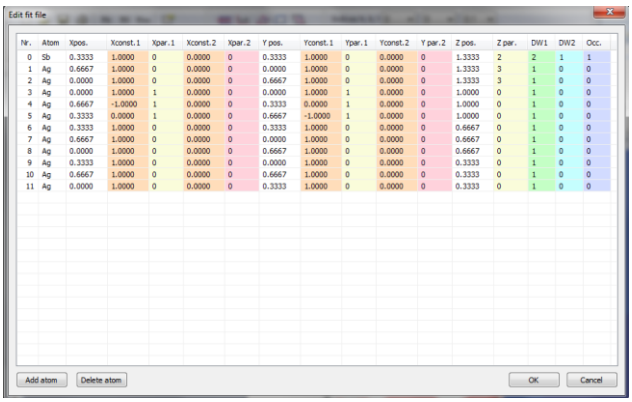
1) Read all important files with extensions *.bul (bulk file), *.fit (fit file for surface modeling), *.dat file with experimental structure factors and *.par (file with parameters).
   In examples directory you can find AgSb and 2012 directories with real data, the AgSb is more simple it has one domain and 2012 has three rotational domains.



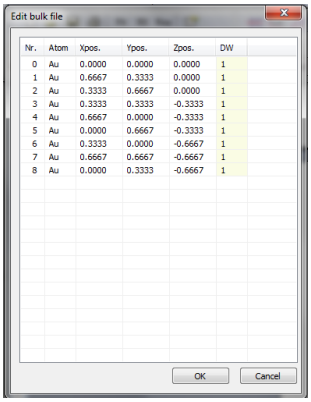
2) When all important files are read the status bar will looks like below:



3) After that you can edit the *.fit or *.bul files, add or remove atoms, add/remove or change parameters. The philosophy is the same like in Rod program. all the changes are directly presented in the 3D model window.

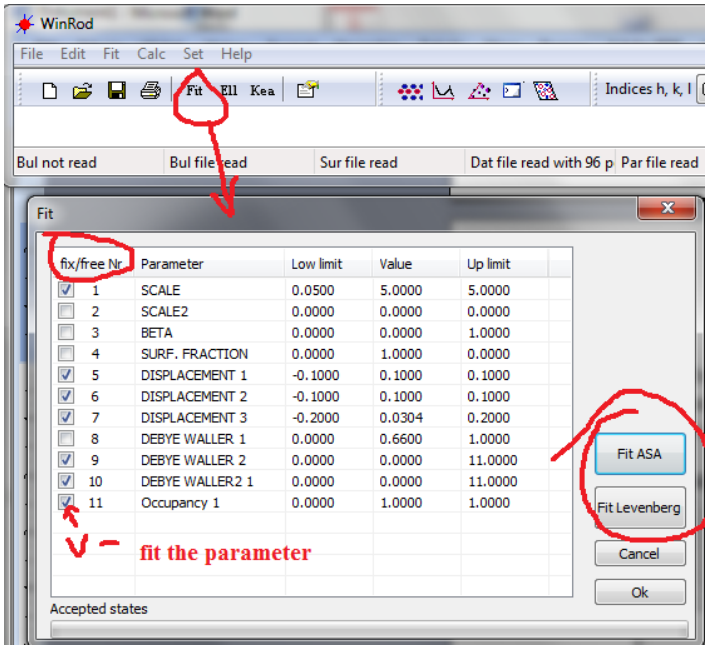


Fit file edit window

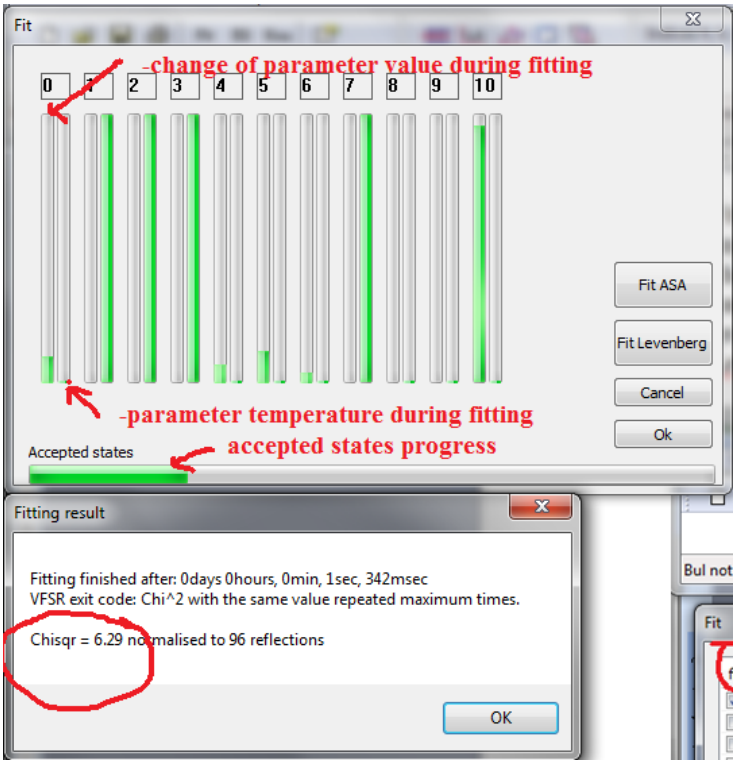


Bul file edit window

4) Fitting is very simple just remember about correct parameter range (not all tests are implemented at the moment and the program is still a bit sensitive to incorrect actions. In the toll bar chose fit after that a new window with fitting routine will appear. Chose the parameters you would like to fit, they starting value and range (after editing values press enter this mandatory prior to accept the change). If all changes are applied press Fit ASA or Fit Levenberg button. This will start the fitting procedure. In WinRod the fitting with ASA is divided on 4 threads (the number can be changed with time if necessary for modern processors) this greatly reduces the calculation time. The advanced processor commands SSE are used only by memory copy provided by Microsoft macros but in a future they can be implemented in Fourier transform what should increase the speed of factor 4.



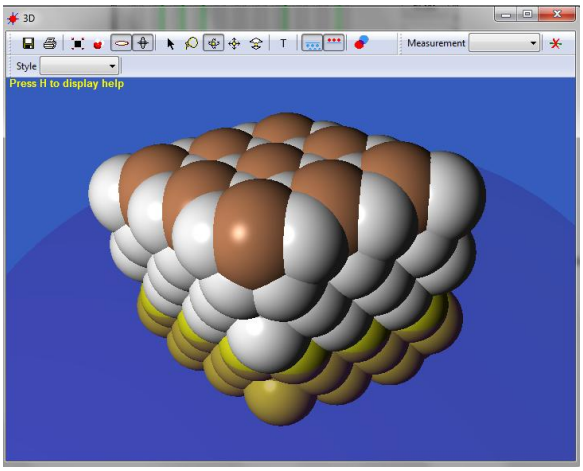
5) Fitting:



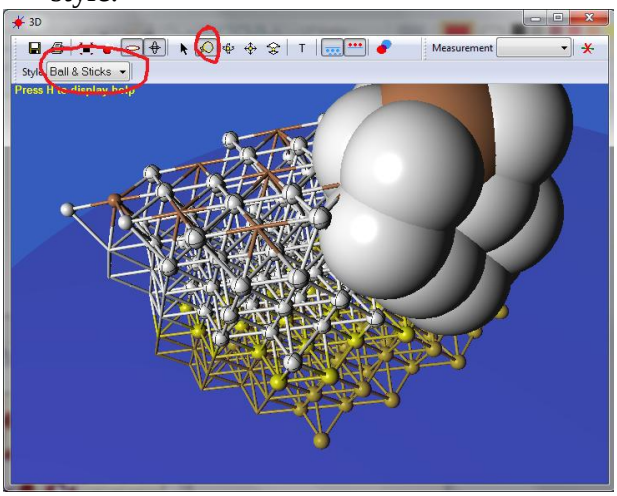
The final result and fitting time is presented in the new window. The χ value is normalized to all data points. Usually for simple problems it takes below 1s. The fitting ASA routine is now hardly optimized for surface diffraction analysis. This was done with specially prepared macros where all fitting parameters were tested in all combinations. After that about 1000 fits were analyzed for the best settings.

6) The 3D model Window can presents results in different ways:

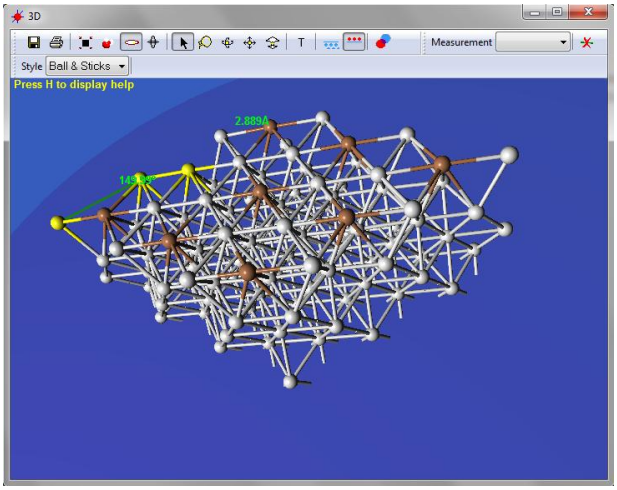
-Standard view



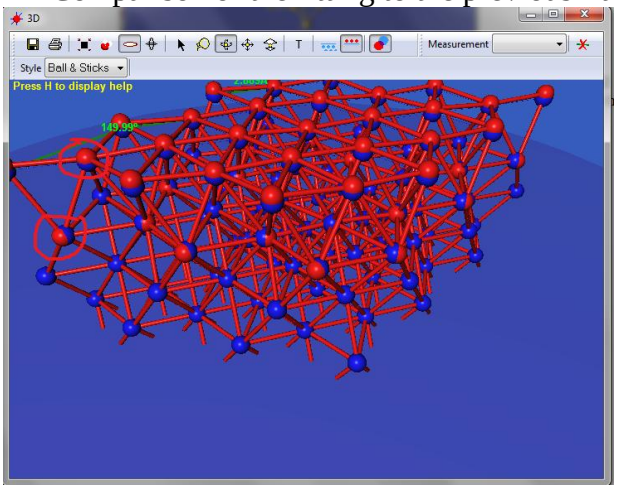
- The list of different styles can be chosen from the marked control. The styles can be mixed by using the select control (smaller ring) and then appropriate presentation style.



Measuring: you can measure distance, angle and torsion angle. First select all interesting atoms and chose the measurement. For distance select two points, for angle three for torsion four atoms.



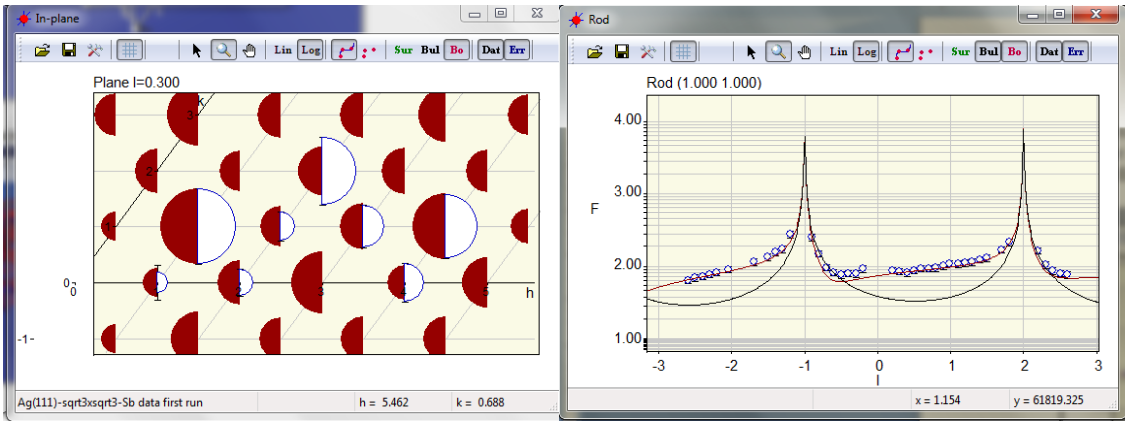
Comparison of the fitting to the previous fit or parameters set.



-Selected atoms can be deleted by spacebar (in this version).

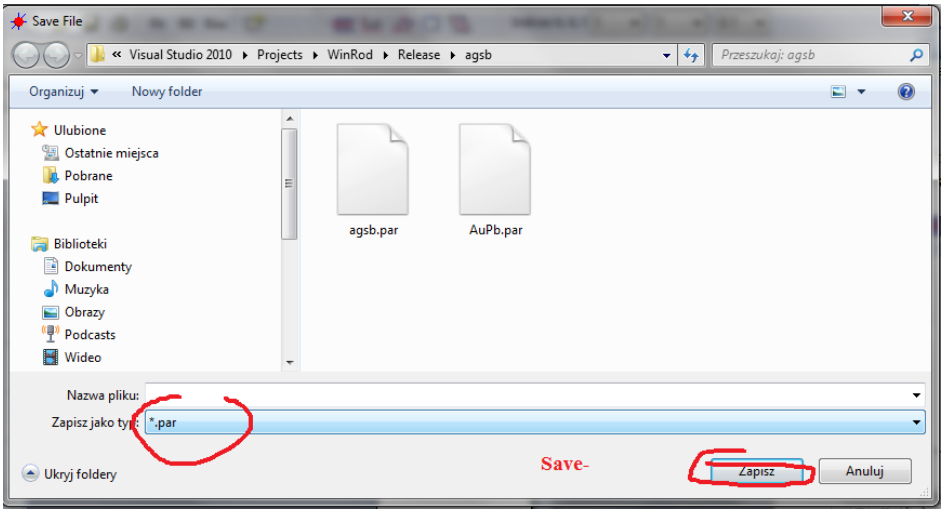
7) Presentation:

-The fitting results are presented in 2D windows: Rod, In-plane and electron density profile in *z* direction. These windows are calculated directly after reading and fitting.

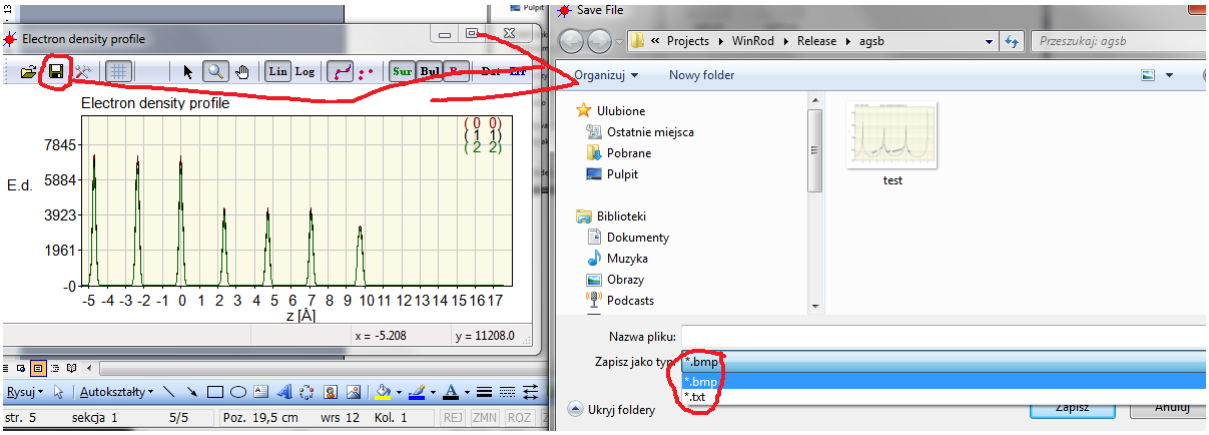


8) Saving and export the results:

-parameter, bulk and fit files can be exported from the main window, at the moment they are not implemented in command line window (the link is there but not fully implemented) and from macro file.

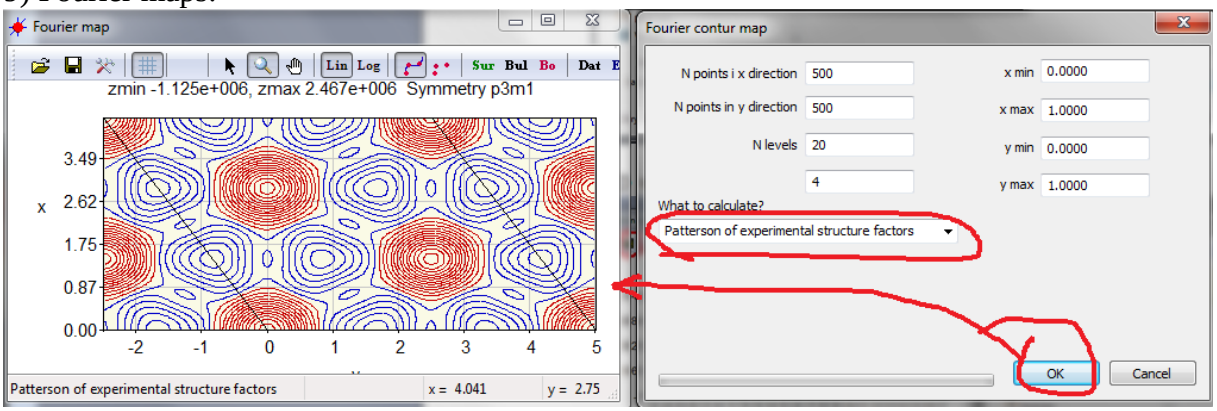


- 2D windows:

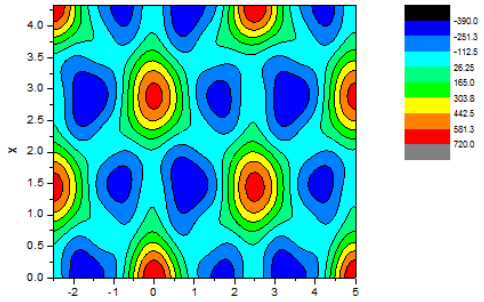


In this case the result can be saved as a bitmap or numerical text file with *x*,*y*,*z* columns. In 2D windows it is possible to change the scale with track ball of the mouse, shifts the scale with the hand tool, zoom it with zoom tool. Pressing the right mouse button sets the most optimal scale calibration. The l range can be also changed from the calc\Rod, In-plane menu.

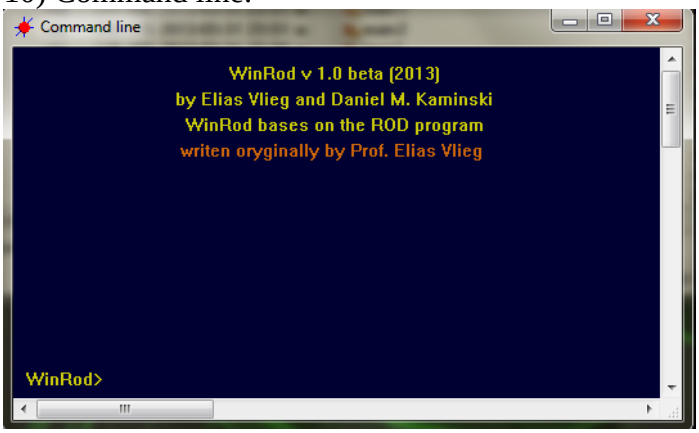
9) Fourier maps:



You have to select what kind of Fourier map to calculate, the *x*, *y* range of calculations, density of calculated points and number of layers. Also in this case it is possible to export numerical data to e.g. Orygin 8.6 and then from this program generate Fourier maps like the one below. The position on the map is shown in status bar on the window bottom.



10) Command line:



Only part of the original functions from Rod is now implemented in the command line. This are: ca (calculate), re – read, set and list.

ca -> ?, inp, rod

set ->list the parameters
list -> bul, sur
plot will is removed completely because is handled by the main program.

11) Macros

In WinRod you can use macros like this one. They can be read from the standard read window:
Example of the parameter file:

```
//Set the parameters
set
indexh 1
indexk 1
indexl 0.2

//Set the parameters for fit engine of ASA
TEMPERATURE_RATIO_SCALE 1.0E-6
TEMPERATURE_ANNEAL_SCALE 1000
COST_PARAMETER_SCALE 0.8
ACCEPTED_TO_GENERATED_RATIO 1.0E-11
INITIAL_PARAMETER_TEMPERATURE 10
DELTA_X 1.0E-7

//Read files
read fit agsb.fit
read bul ag111.bul
read dat agsb.dat

read par agsb.par

//Fit the data and repeat the fitting  50 times
fit loop 50
fit asa
fit run
```