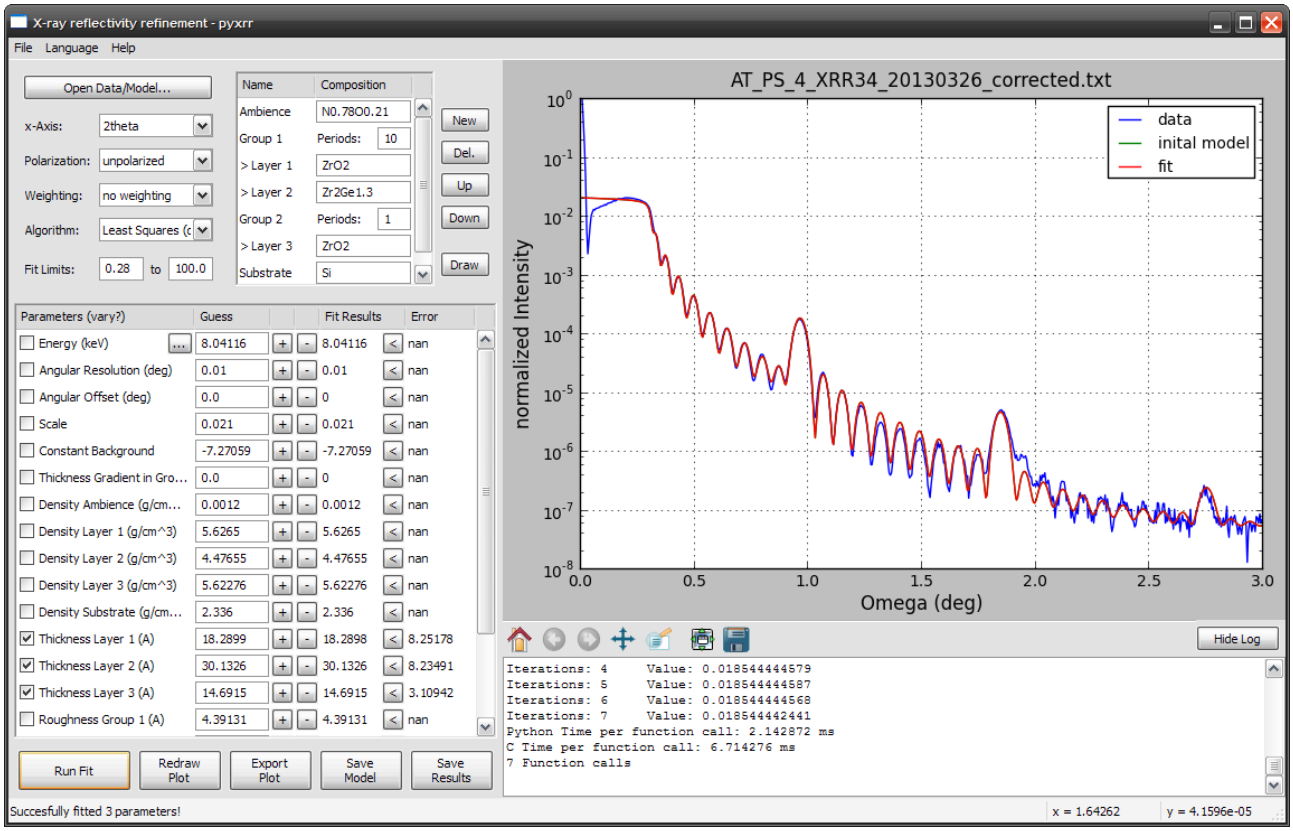
Introduction to pyxrr_GUI

This is a short introduction to the usage of the graphical user interface (GUI) that was developped to simplify the usage of pyxrr. Further details regarding pyxrr can be found in the pyxrr manual (see "manual.pdf" in the pyxrr folder).

Installation of pyxrr_GUI is only relying on the proper installation of pyxrr (with which pyxrr_GUI is distributed). This is easily achievable by downloading the latest pyxrr package and following the instructions found in "install.txt".

To start pyxrr_GUI simply execute "pyxrr_GUI_v0.6.pyw" found in the contrib folder. A typical screen (data already loaded) is depicted in the following:



The menu:

- The file menu allows to execute all operations that are found as buttons on the GUI. Also it shows the keyboard short-cuts for these operations.
- The language menu allows to switch between German and English user interface. This reloads the complete window.
- The help menu just shows some short information on the program.

The structure of the user interface:

- On the top left a button to import measured data or a pyxrr model file is found. This is usually the first thing to do. Underneath, following settings are found:
  - x-axis of the measured data (as saved in the loaded file),
  - polarization of the X-ray beam (typical X-ray tubes provide unpolarized radiation),

    - weighting of the data applied during the fitting (usually set to none),
    - algorithm used for fitting (usually "Least Squares" is the fastest option),
    - fit limits for omega (the fit curve is always plotted for the complete measuring range).
- In the center, a list showing the layer model is found:
    - The topmost layer is always Ambience (typically air, i. e. $N_{0.78}O_{0.21}$) and the bottom layer is always the substrate.
    - In-between, groups of layers can be inserted, deleted and moved with the small buttons right to the list box. A group can be a multi-layer by increasing the number of periods.
    - The materials are simply entered in the text boxes using element symbols and numbers for stoichiometry.
    - The button "Draw" gives a plot of density over thickness for the model.
- The lower left provides a list of model parameters and the main user buttons:
    - Activating a check box left to a parameter will fit this parameter during the next refinement.
    - After setting up the layer model, all parameters found in the text boxes should be set. Usually, you should go through the complete parameter list and adjust everything to your measurement and sample. Pressing Enter in a textbox updates the graph.
    - After running a refinement (using the "Run Fit" button or Ctrl+F), refined values and estimated errors are displayed. The buttons "<" are used to load the fitted values in the textboxes. The buttons "+" and "-" adjust the textbox values and update the graph.
    - The button "Save Model" saves all parameters and a link to the data file in a pyxrr model file. This can be loaded directly by the open dialogue.
    - The button "Save Results" creates a text file with all starting parameters, the fitting results and errors as well as three columns of data: omega, measured data, fit data.
- In the top right, the graph displaying data, starting model and fitted model is displayed. The usual matplotlib toolbar can be used to switch between move and zoom mode in the graph.
- The lower right shows a log window with all the output generated by pyxrr. It can be disabled by pressing the button "Hide Log".
- The statusbar displays some messages and x-y-coordinates when hovering the graph.

Have a lot of fun!