Rietveld Program Manual

* You first have to change the path where you have copied the Rietveld folder in the inipath.m file

*rvpath = fullfile('C:', 'Users', 'hrp', 'Documents', 'MATLAB', 'rietveld');*

* After starting matlab, you have to enter the following command to initialize java

*javaaddpath('C:\Users\hrp\Documents\MATLAB\rietveld\base\gui\RietveldGUI\dist\RietveldGUI.jar',1)*

* To get the program ready you have to initialize the file init.m with the following command

*script.init*

* In this script you define how many spectrums you want to analyze and which modules you want to use (you only have to change the number of spectrums here, analyze 30 Spectrums at once seems to work best: numberOfSpecs = 30)
* Then you have to initialize the Input script to load all the structural parameters and start parameters as well as the information about the measurement (like twotheta, ringcurrent, deatime etc.) e.g.:

*script.TiH2\_InputScript\_cubic\_TiH2\_PSART40*

* You’ll find the scripts in the Script folder
* Then you load the gui with the following command:

*rietveld.gui.ParameterEditor*

* The gui opens
* Before you do anything you have to initialize the data
* You do this by entering “rc” in the field: “Rietveld-Container-Name in work space”
* To load the data from the Input script you initialized before you press the button “Import from Workspace”
* The next thing You do is entering the boundaries (lower and upper) for the data points in the spectrum
* The numbers are the channel numbers because the channel to energy conversion is done in the program
* You can search for this parameter by searching the gui for “lo” – then the parameter “LowerChannelBound” should appear, here you enter the first Channel number
* After this you enter the last channel number in the field “UpperChannelBound”
* Then you export the information to the workspace by clicking the button “Export to Workspace”
* Then you have to initialize the Channel-to-Energy vonversion by entering this command:

*rc.computeEnergyData*

* Then you go back to the gui and import the new data from the workspace
* Now all the data is prepared and you can start the refinement
* In the gui you can change which parameter should be refined and which should be constant, just by clicking on the “refinable” button so that it is marked with a tick
* After you change a parameter to be refined you have to export the data to workspace again
* To start the fitting you enter this command:

*fitter.executeFit(rc);*

* Then the fitting starts
* When it’s done you go back to the gui and import the fitted data from workspace
* In the gui you also have the opportunity to change the format from “use all parameters”, where you have listed each parameter of each spectrum to “use each parameter once”
* This makes it easier to refine the parameters of all spectrums at once
* To plot the spectrums you use the following command:

*rietveld.gui.Plot(analysis)*