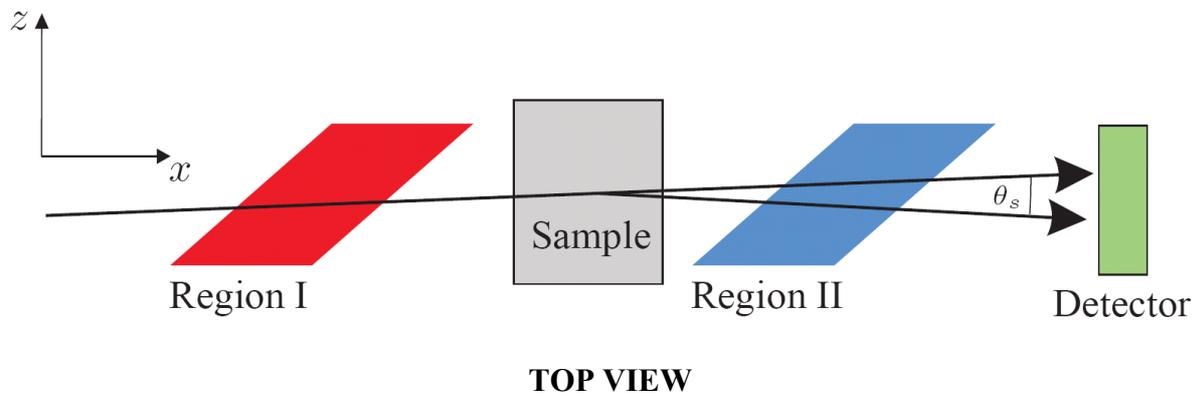


SENRef User's Guide

V1.1



V.O. de Haan

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1. Introduction

The acronym *SENRef* represents the words *Spin Echo Neutron Reflection*. Hence, the program was designed to interpret these kinds of measurements. Such measurements can be performed either in Time-of-Flight (TOF) mode or in monochromatic mode. In TOF mode the incident angle is fixed and in general a position sensitive detector (PSD) is used as a neutron counting device. The wavelength (λ) of the neutrons is determined by the time it takes for the neutron after passing the chopper to reach the detector. In this time slot the neutrons will have interacted with the sample surface, either by refraction, specular reflection or off-specular reflection. In monochromatic mode the wavelength of the neutrons is fixed to some small interval and the incident angle is varied. The angle after interaction with the sample can be determined, either by a PSD or by a slit in front of a single detector. The definition of the sample geometry is given in figure 1.

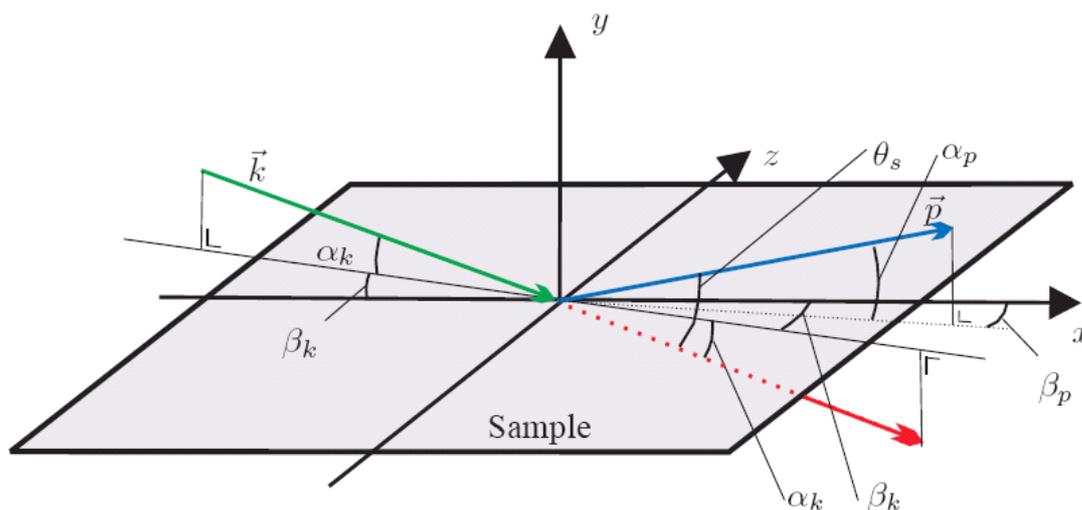


Figure 1: Definition of angles in spin echo neutron reflection geometry. α_k is the angle between the path of the incident neutron (represented by vector \vec{k} , indicated by the green arrow, or the red arrow where the start of the vector has been shifted to the sample surface) and the sample surface. β_k is the angle the path of the incident neutron makes with the xy -plane. α_p the angle between the path of the off-specular scattered neutron (vector \vec{p}) and the sample surface and β_p is the angle between the path of the off-specular scattered neutron and the xy -plane. θ_s is the angle between the path of the off-specular scattered neutron and the path of the not-scattered neutron.

In general the wave vectors are given by:

$$\vec{k} = \frac{2\pi}{\lambda} \begin{pmatrix} \cos(\alpha_k) \cos(\beta_k) \\ -\sin(\alpha_k) \\ \cos(\alpha_k) \sin(\beta_k) \end{pmatrix} \quad \vec{p} = \frac{2\pi}{\lambda} \begin{pmatrix} \cos(\alpha_p) \cos(\beta_p) \\ -\sin(\alpha_p) \\ \cos(\alpha_p) \sin(\beta_p) \end{pmatrix}$$

Throughout the program the small angle approximation for the determination of the wave vectors is used, hence

$$\vec{k} = \frac{2\pi}{\lambda} \begin{pmatrix} 1 - \frac{1}{2}(\alpha_k)^2 - \frac{1}{2}(\beta_k)^2 \\ -\alpha_k \\ \beta_k \end{pmatrix} \quad \vec{p} = \frac{2\pi}{\lambda} \begin{pmatrix} 1 - \frac{1}{2}(\alpha_p)^2 - \frac{1}{2}(\beta_p)^2 \\ -\alpha_p \\ \beta_p \end{pmatrix}$$

The neutron beam of a reflectometer is always collimated in two directions. The first direction, parallel to the sample surface is in general very wide, and the second direction perpendicular to the surface is in general small, some mm to 1/10 of mm. The latter slit width is important for the resulting profile resolution and determines also the coherence length of the neutron beam along the sample surface. The former slit width is kept wide to keep the beam intensity as high as possible as the reflected intensity will be orders of magnitude smaller than the incident intensity (as much as 6 to 8 orders have been achieved).

The Spin Echo technique can be used to code a component of the direction of an individual neutron in the beam and find out the component of the scattering angle in the same direction¹. If this direction is used along the wide slit direction, then also the scattering angle parallel to the sample can be determined, yielding information on the sample surface in all directions. The information obtained in the direction parallel to the surface are the sample surface correlation functions and perpendicular to the surface the sample profile².

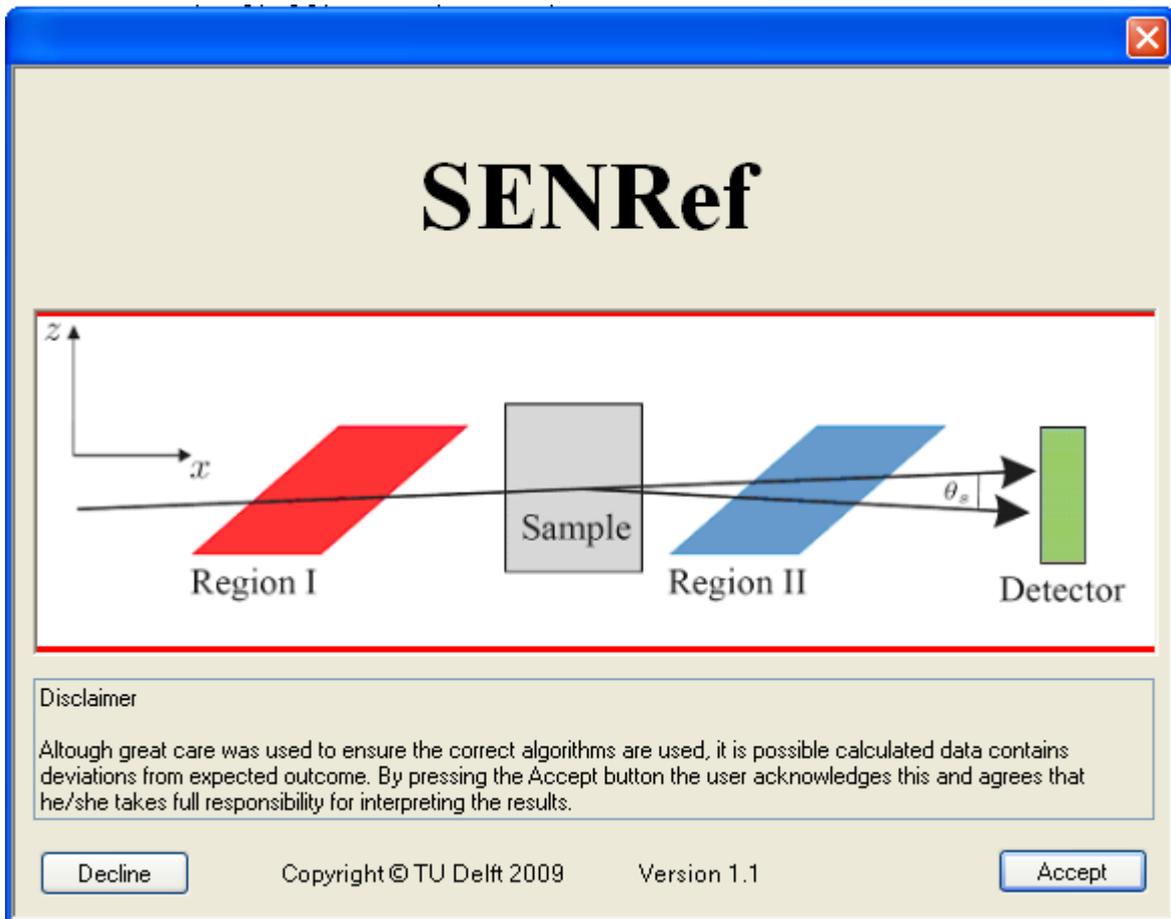
¹ J. Plomp, "Spin-echo development for a time-of-flight neutron reflectometer", Thesis Delft University of Technology, 2009

² V.O. de Haan, "Coherence approach to neutron propagation in spin echo instruments", 1st ed, BonPhysics Research and Investigations B.V., 2007.

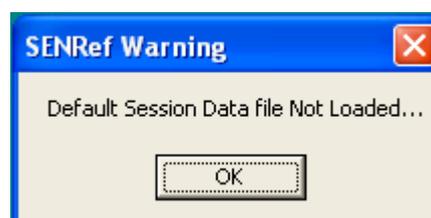
2. Start program

The program is written in Microsoft Visual Studio 2005 (Visual Basic) and will need the .NET Framework. This will all ready be installed on your computer, installed at set-up, or you should provide it yourself.

When the program is started a splash screen will pop up showing a disclaimer you have to accept before the program continues:



Push the Accept button if you agree that the use of the program is at your own risk and no rights or claims can be derived from using the program. If this button is pressed the program continues, searching in the resources sub directory of the directory where the program is stored, for a XML-formatted file that contains the default settings. If the program can not locate the file in this directory, the user is prompted by a file input dialog box typical for the operating system to indicate where the file can be found. The user can select a session data file or press the *CANCEL* button. If this button is pressed the program issues a warning, indicating that no session data file was loaded:



After pressing the OK button the program continues with the default values of the program. The above *SENRef Warning* dialog box will appear whenever the user does something unexpected.

For all parameters tooltips are given, explaining shortly the use of the control that is pointed at with the mouse.

The program has a button driven interface which consists of 1 tab control with 7 major tab windows: *Instrument*, *Sample*, *QxQyPlot*, *QxCuts* and *QyCuts*, *Fitting* and *Thanks* and three buttons *Load Session*, *Save Session* and *Make Session Default*.

Load Session button

This button enables the session data input. If pressed a file selection dialog will pop up requesting a filename. The used extension is XML as the session data file is XML formatted. If a valid filename is chosen the session data file will be loaded, enabling the continuation of a previous session.

Save Session button

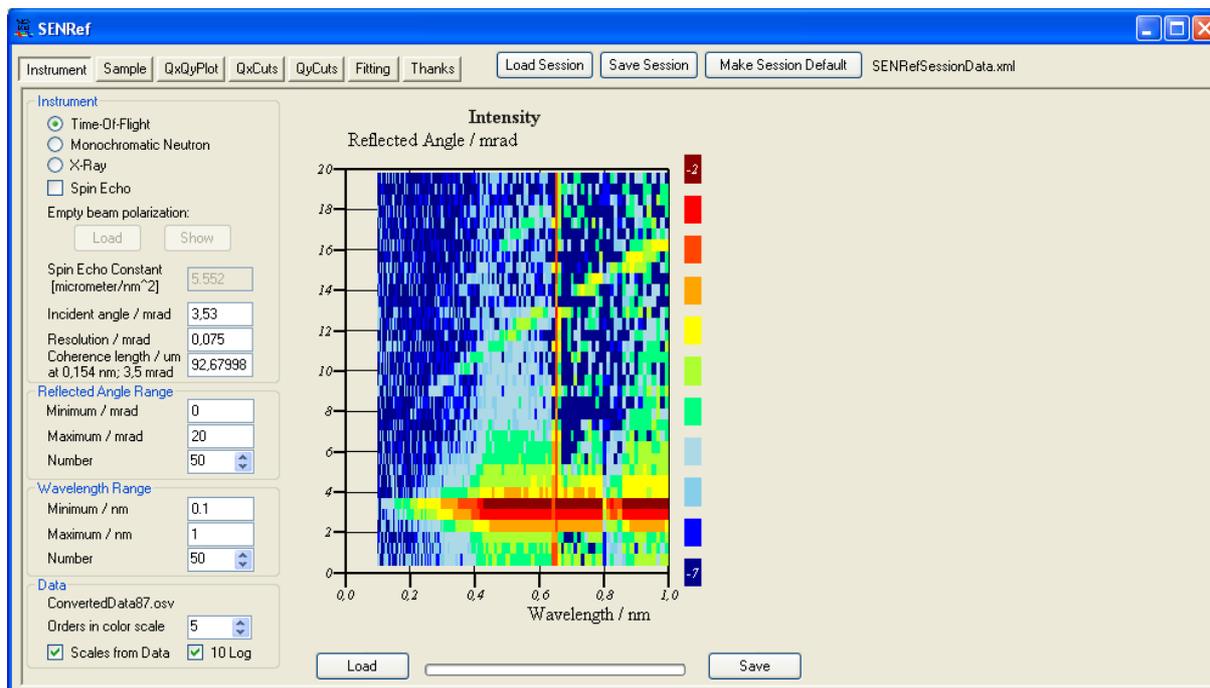
This button enables the session data output. If pressed a file selection dialog will pop up requesting a filename. The used extension is XML as the session data file is XML formatted. If a valid filename is chosen the session data file will be saved, enabling the continuation in a future session.

Make Session Default button

This button enables the creation of a default session data file. If pressed the session data is saved in the default session data file that will be automatically loaded at the next start of the program.

Clicking the names of the tab windows will select that window. The Instrument Window is used to define the instrument parameters and load the measured data. The Sample Window is used to define the sample parameters, load sample profiles and perform calculations. The QxQyPlot, QxCuts and QyCuts windows are used for diagnostic purposes and defining the cuts. These windows work for either or both the loaded data, including the calculation of the error bars (for QxCuts and QyCuts), and the calculated data. The Fitting window can be used to fit the selected sample model to the data. The Thanks windows contains clickable images yielding information about the program and theory behind the calculations used.

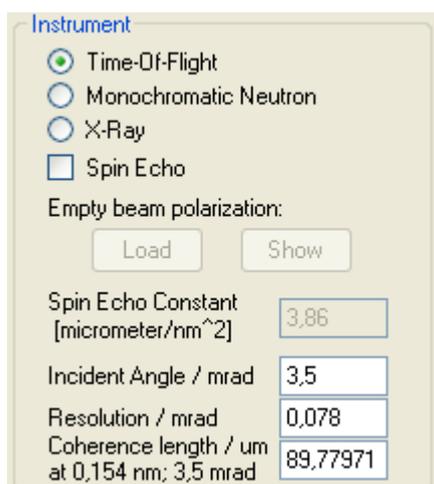
3. Instrument Window



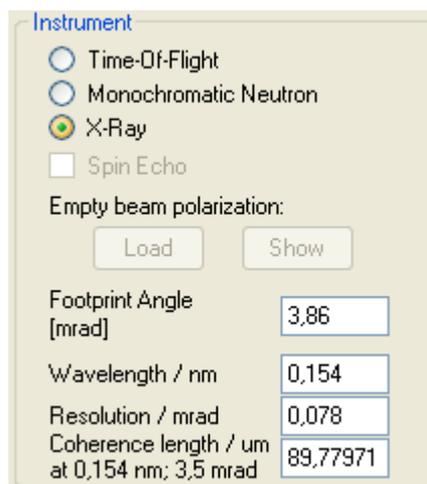
To the left the Instrument Window has 4 panels: *Instrument*, *Reflected Angle Range*, *Wavelength Range* (or *Incident Angle Range*) and *Data* panel. To the right there is space for viewing the data after loading. Depending on the status of the instrument panel and the data loaded, graphs are given of the relevant neutron or X-ray intensity plots. At the bottom there are two buttons: *Load* and *Save*.

Instrument panel

Time-Of-Flight mode:



Monochromatic mode:



The instrument panel consists of three selection boxes for the measurement type and a check box for the *Spin Echo* mode, four input boxes *Spin Echo Constant* (or *Footprint angle*), *Incident Angle* (or *Wavelength*), *Resolution* and *Coherence length* and a *Load* and *Show* button.

Selection boxes measurement type

Select either Time-of-Flight (only for neutron scattering), Monochromatic Neutron or Monochromatic X-Ray. In Time-of-Flight mode the second input box on the instrument panel changes to the input box for the Incident Angle. In monochromatic mode it changes to the one for the Wavelength. The first input box changes from Spin Echo Constant in Time-Of-Flight mode into Footprint Angle in monochromatic mode. In Time-of-Flight mode the 3rd panel from the top changes to the Wavelength Range panel. In monochromatic mode it changes to the Incident Angle Range panel.

Check box Spin Echo

In Time-of-Flight mode, it is possible to indicate whether the measurements are made with Spin Echo or without. Without Spin Echo only the non-polarized scattered intensity can be calculated or loaded / saved. With Spin Echo the plus and minus scattered intensity can be calculated or loaded / saved. As an extra in the Spin Echo mode, the polarisation and the shim intensity can be shown. Further the input box *Spin Echo Constant* and the *Load* button will be enabled.

Input box Spin Echo Constant

In Time-Of-Flight mode the spin echo constant is used. The input must be changed to the desired value and depends on the setting of the apparatus. The value represents the spin echo length in micrometers divided by the square of the wavelength of the neutrons in nanometres.

Input box Footprint Angle

In Monochromatic mode the spin echo constant is not used, but the footprint angle is important. The value represents the incident angle at which the incident beam just covers the sample length in the direction of the beam. For larger incident angles the beam footprint is reduced with the ratio $\sin(\text{Footprint angle}) / \sin(\text{Incident angle})$ and the intensity with the square of this ratio. The input must be changed to the desired value and depends on the setting of the apparatus.

Input boxes Incident Angle (or Wavelength), Resolution and Coherence length

These inputs must be changed to the desired values. The Incident Angle is the angle between incident beam and sample surface. The resolution is the standard deviation of the Gaussian distributed Incident Angle spread of the beam. The coherence length is the width of a homogeneous, Gaussian distributed, mutual coherence function. As the three variables are coupled (see chapter 6.1.1 of reference in footnote 2) changing one will result in a corresponding change of the others. For SENRef the relation between these parameters is:

$$r_c = \frac{\lambda}{2\pi} \frac{1000}{\alpha_k \Delta\alpha_k},$$

where r_c is the Coherence Length in micrometer units, λ the Wavelength in nanometer, α_k the Incident Angle in milliradians and $\Delta\alpha_k$ is the Resolution also in milliradians.

Load button

This button enables the empty beam polarization input. If pressed a file selection dialog will pop up requesting a filename. Extensions are OUT (for a space delimited file), OSV (for a TAB delimited file) or CSV (for a comma delimited file). The format of the input file is defined in appendix B. If a valid filename is chosen, another window will pop up enabling the correct data input. This window is called *Import Data File Window* (See also the Load Button on the Grating Data panel on the Sample Window).

Show button

The Show button enables investigation of the loaded empty beam polarization. If this button is pressed a window will pop up showing the data. This window is called *Show Data Window* (See also the Load Profile Button on the Sample Window).

Reflected Angle Range panel

Reflected Angle Range

Minimum / mrad	0
Maximum / mrad	20
Number	50

This panel consists of three input boxes: *Minimum*, *Maximum* and *Number*. They define the linear range and step over which the reflected angle is varied. This range will be used for the calculations if the *Scales from Data* selection box is *not* checked.

Incident Angle Range panel (Available when in Monochromatic Mode)

Incident Angle Range

Minimum / mrad	0
Maximum / mrad	20
Number	50

This panel consists of three input boxes: *Minimum*, *Maximum* and *Number*. They define the linear range and step over which the incident angle is varied. This range will be used for the calculations if the *Scales from Data* selection box is *not* checked.

Wavelength Range panel (Available when in Time-Of-Flight Mode)

Wavelength Range

Minimum / nm	0.1
Maximum / nm	1
Number	50

This panel consists of three input boxes: *Minimum*, *Maximum* and *Number*. They define the linear range and step over which the wavelength is varied. This range will be used for the calculations if the *Scales from Data* selection box is *not* checked.

Data panel

This panel consists of one input box, one output box and two selection boxes. The input box is a number to change the logarithmic colour scale of the graphs. The output box is only visible when a data file has been loaded and shows the name of the data file. The selection boxes are the *Scales from Data* selection box and the *10 Log* selection box:

Scales from Data selection box

If selected (checked) the calculation scales are the same as the data scales. If not selected the calculation scales are as defined on the Instrument Window.

10 Log selection box

If selected (checked) the colour plot scale is logarithmic with base 10. If not selected the scale is linear.

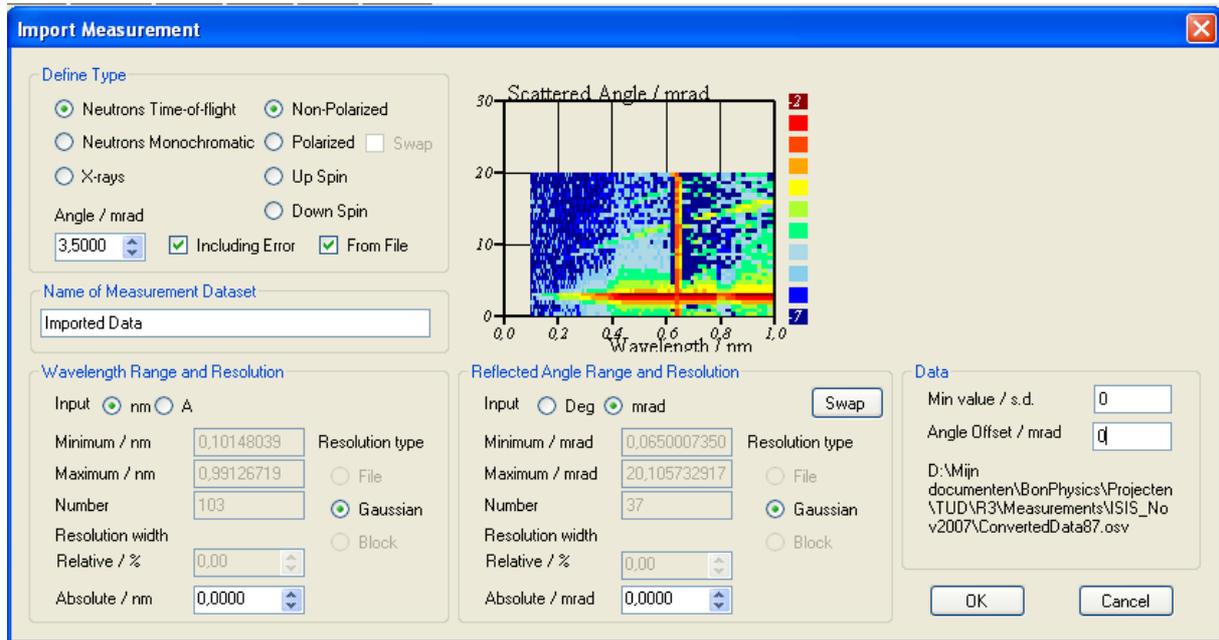
Save button

This button enables the data output. If pressed a file selection dialog will pop up requesting a filename. Extensions are OUT (for a space delimited file), OSV (for a TAB delimited file) or CSV (for a comma delimited file). If a valid filename is chosen the data will be saved under that name. The format of the file is the same as of the input file (see Appendix A), but errors will not be included.

Load button

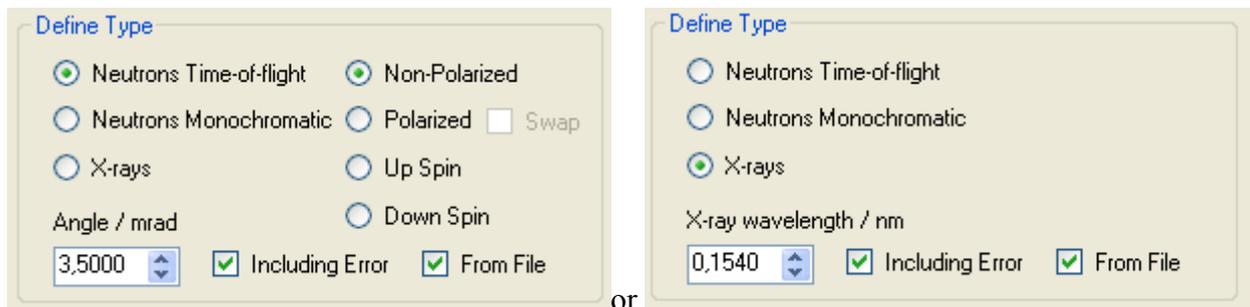
This button enables the data input. If pressed a file selection dialog will pop up requesting a filename. Extensions are OUT (for a space delimited file), OSV (for a TAB delimited file) or CSV (for a comma delimited file). If a valid filename is chosen another window will pop up enabling the correct data input. This window is called *Import Measurement Window*.

4. Import Measurement Window



To the upper left the window has two panels: *Define Type* and *Name of Measurement Dataset*. To the upper right there is space for two graphs, showing the selected input data. At the bottom there are three panels: *Wavelength Range and Resolution* (or *Incident Angle Range and Resolution*), *Scattered Angle Range and Resolution* and *Data*. Finally at the right bottom of the window there are two buttons *OK* and *Cancel*.

Define Type panel

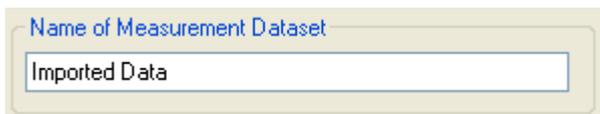


This panel is used to select the type of data that is loaded with the selected file. The data file is very simple, not containing this information. Initially the values are copied from the Instrument Window. To the left side the panel consists of selection type buttons comparable with the ones used in the Instrument panel and an input box for the incident angle or wavelength depending on the selected measurement type. To the right side one can select which data is included in the selected file. The format of the input file is defined in appendix A.

If the selection box *Polarized* is checked, the selection box *Swap* is enabled. The box interchanges the plus and min intensity, inverting the resulting polarization.

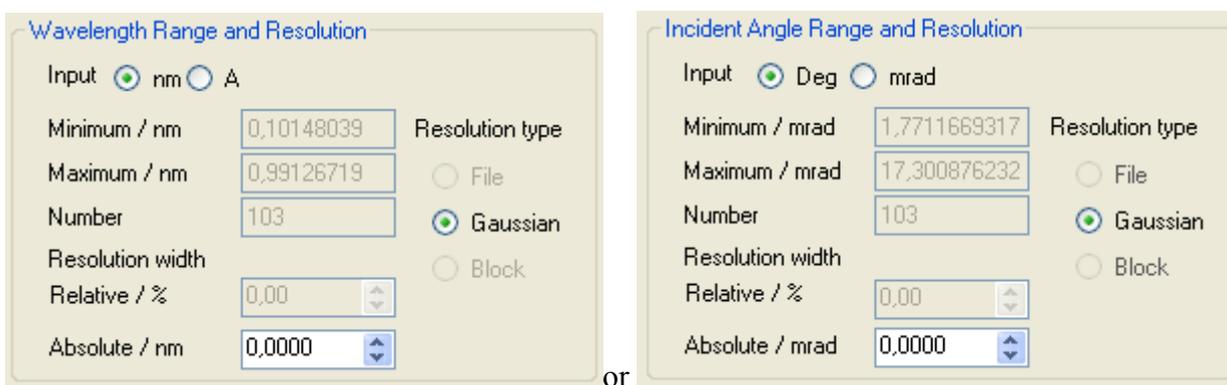
If the selection box *Include Error* is checked the selection box *From File* will be enabled. If both selection boxes are checked the program expects the data to contain the errors, according to the format of appendix A. If the selection box *From File* is not checked, but *Including Error* is, the program assumes that the data in the file are raw neutron counts and the error is calculated as the square root of the counts. If selection box *Including Error* is not checked, all errors are set to 0.

Name of Measurement Dataset panel



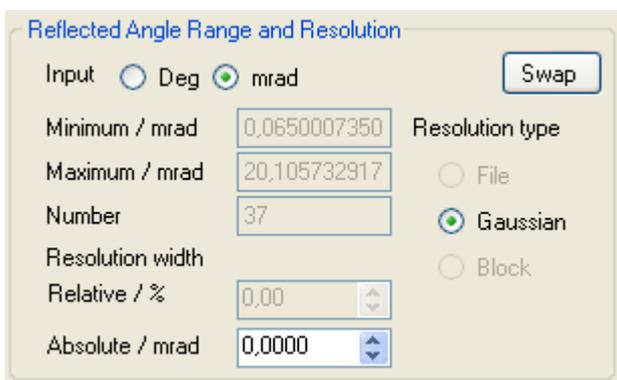
This panel contains an input box for the name of the loaded dataset. It can be used for future reference.

Wavelength or Incident Angle Range and Resolution panel



This panel contains 2 selection criteria: Input (nm or A) and Resolution type (File, Gaussian and Block), three output and two input boxes. *Minimum*, *Maximum* and *Number* define the range and number of data points in the data file. *Relative* and *Absolute* define the resolution distribution (not used for now).

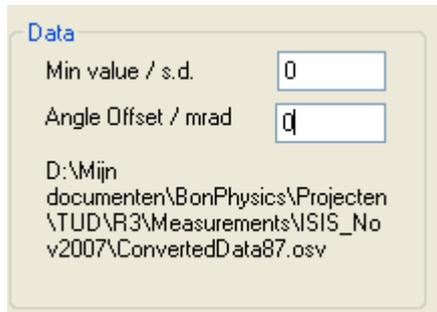
Scattered Angle Range and Resolution panel



This panel contains 2 selection criteria: Input (Degrees or milliradians) and Resolution type (File, Gaussian and Block), three output and two input boxes. *Minimum*, *Maximum* and *Number* define the range and number of data points in the data file. *Relative* and *Absolute*

define the resolution distribution (not used for now). The button Swap at the upper top side is used to swap the data in the file so that the axes are interchanged.

Data panel



This panel consists of two input boxes and an output box. The output box shows (part of) the data file name. The input box *Min value* is enabled if the *Including Error* box was selected in the Define Type panel. If the relative error of the data point is larger than the value in this box, the error is set to 0. The input box *Angle Offset* is used to shift the incident angle scale over the value given in the box.

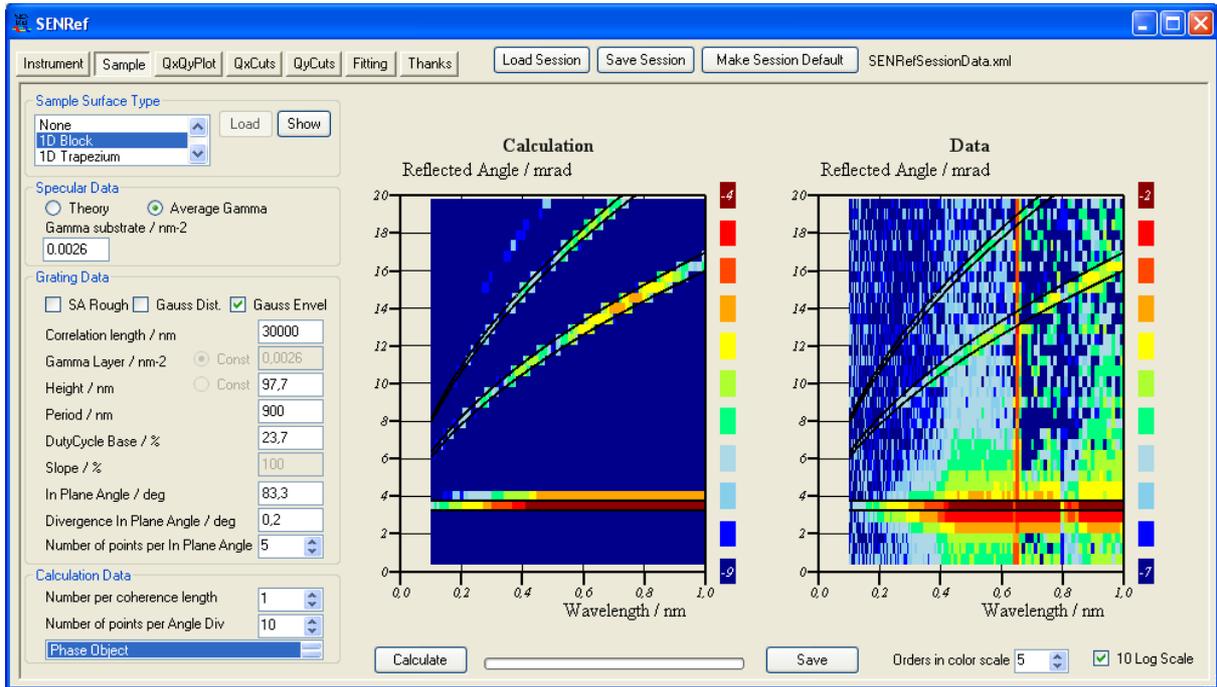
OK button

This button copies the data to the main program and returns the control to the Instrument Window.

Cancel button

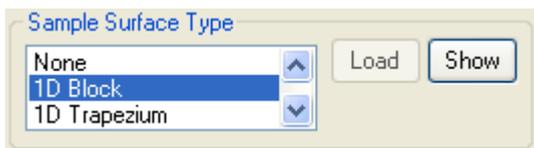
This button ignores the data and returns the control to the Instrument Window.

5. Sample Window



To the left side this window has four panels: *Sample Surface Type*, *Specular Data*, *Grating Data* or *Isotropic Data* (or nothing) and *Calculation Data*. To the right side it has a selection box *Type*, two output graphs, two buttons *Calculate* and *Save*, an input box *Orders in colour scale* and a selection box *10 Log Scale*. The panel *Grating Data* appears if a 1D or 2D profile is selected. The panel *Isotropic Data* appears if an Isotropic profile is selected.

Sample Surface Type panel



This panel defines the type of profile or correlation function describing the sample. From this function the scattering is calculated according to the approximation selected in the *Calculation Data* panel. The panel has one selection box and two buttons and an output box.

Selection box

Several predefined sample surface types can be selected. An 1D or 2D surface type is described by a height profile. An isotropic sample surface type is defined by a Gaussian correlation function. The formula used depends on the selected approximation and is given in Appendix C. The profile or correlation can be predetermined or user defined.

Capillary Waves selection

The Gaussian roughness correlation function is given by:

$$C(r) = \sigma^2 \left(1 - \frac{r_{\min}}{2\xi} \ln \left(\frac{r}{r_{\min}} + 1 \right) \right)$$

where σ is the roughness and ξ the correlation length. See also the reference in footnote 3. The value for r_{\min} is a cut-off value $r_{\min} = a\xi / N$, where

N = value of input box *Number of points per correlation length*

a = value of input box *Integration range in correlation length*

Gravitational Waves selection

The Gaussian roughness correlation function is given by:

$$C(r) = \sigma^2 K_0(r/\xi + \alpha)$$

where σ is the roughness, ξ the correlation length and K_0 the modified Bessel function of zero-the order. See also the reference in footnote 3. The value for $r = 0$ is cut-off for $K_0(\alpha) = 1$ ($\alpha \approx 0.45689248915903589527$).

Self-affine fractional selection

The Gaussian roughness correlation function is given by:

$$C(r) = \sigma^2 e^{-(r/\xi)^{2h}}$$

where σ is the roughness, ξ the correlation length and h the so-called jaggedness parameter. See also the reference in footnote 3.

Self-affine fract (anal) selection

Similar to *Self-affine fractional*, but calculated analytically following the method described by R. Pynn, Phys. Rev. B, Vol.45, No 2, January 1992 p602-612. See also appendix D.

Output box

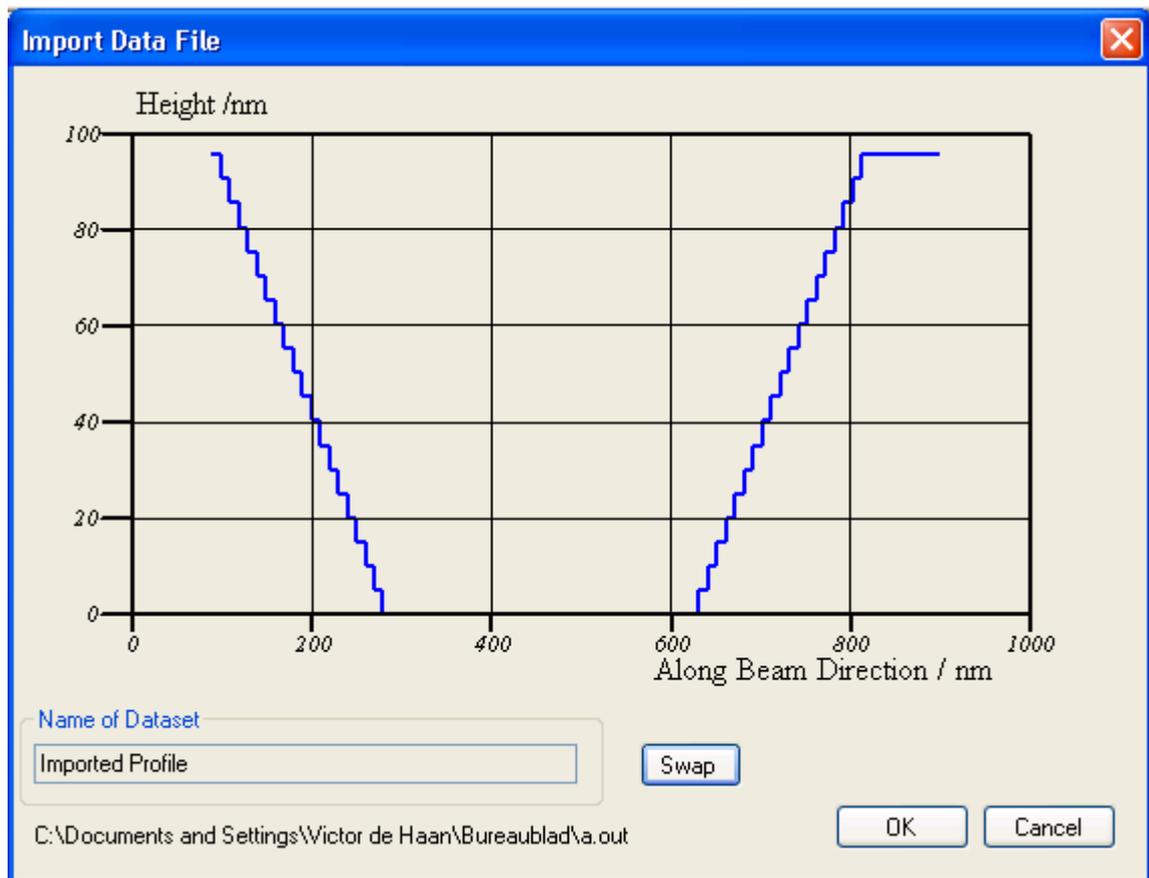
The output box, just below the Load button, shows the filename of the loaded profile (if present, other wise the output box is empty).

If a user defined height profile or correlation is selected, the button *Load* is enabled.

Load button

This button enables the profile input. **Note that for a 1D or 2D user defined profile the height distribution is loaded and for an isotropic defined profile the correlation function.** If pressed a file selection dialog will pop up requesting a filename. Extensions are OUT (for a space delimited file), OSV (for a TAB delimited file) or CSV (for a comma delimited file). The format of the input file is defined in appendix B. If a valid filename is chosen another window will pop up enabling the correct data input. This window is called *Import Data File Window*.

Import Data File Window



At the upper part of the window the data is shown as loaded. To the lower left the window has one panel: *Name of Dataset*. This panel contains an input box for the name of the dataset. It can be used for future reference. Below this panel an output box shows the filename of the imported data. To the lower right it contains three buttons:

Swap button

This is used to swap the data in the file so that the axes are interchanged.

OK button

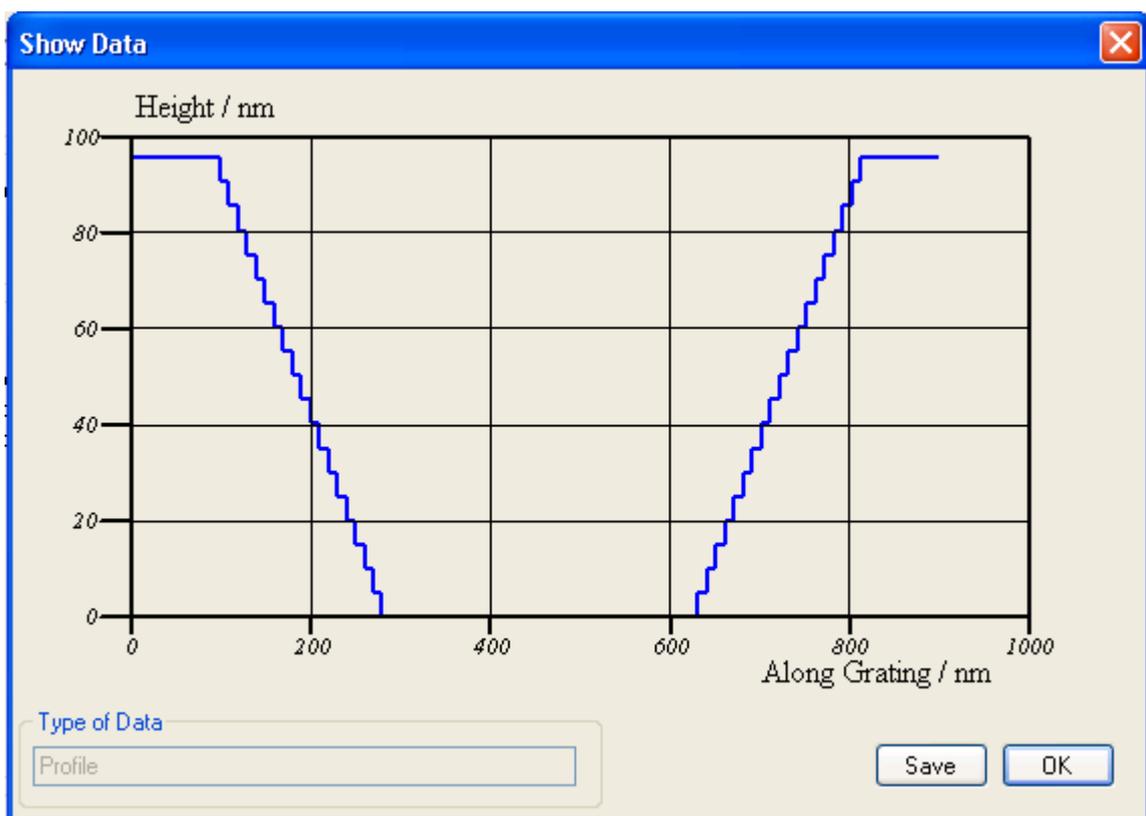
This button copies the data to the main program and returns the control to the Instrument Window.

Cancel button

This button ignores the data and returns the control to the Instrument Window.

Show button

This button presents the used profile. If this button is pressed a window will pop up showing the profile as it is defined. This window is called *Show Data*.



At the upper part of the window the defined profile is shown. To the lower left the window has one panel: *Type of Data*. This panel contains an output box indicating the type of data. To the lower right it contains two buttons:

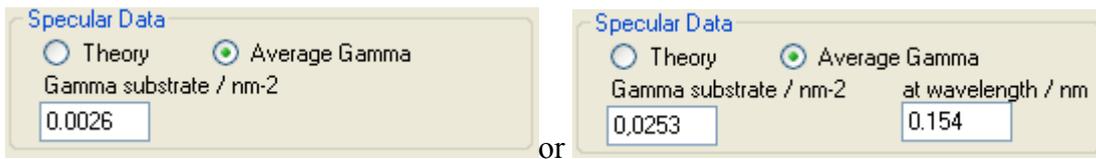
Save button

This is used to save the data into a file. Extensions are OUT (for a space delimited file), OSV (for a TAB delimited file) or CSV (for a comma delimited file). If a valid filename is chosen the data will be saved under that name. The format of the file is the same as of the input file (see Appendix B).

OK button

This button returns the control to the Instrument Window.

Specular Data panel



This panel defines the sample surface and the way the specular part of the reflectivity is calculated. It consists of two selection boxes, *Theory* and *Average Gamma*, and one (or two in X-Ray mode) input box (es) *Gamma* substrate (and *at wavelength*)

Theory selection box

If selected the specular part is calculated from the theory provided by the selected approximation. The formula used is given in Appendix C.

Average Gamma selection box

If selected the specular part is calculated from the scattering length density profile determined by the surface average of the height profile function.

Gamma substrate input box

This value represents the scattering length density of the sample substrate material times 4π in nanometer⁻² units.

at wavelength input box

In X-Ray mode this value represents the wavelength corresponding to the value given for the scattering length density of the sample material in the Gamma input box.

Grating Data panel

The screenshot shows the 'Grating Data' panel with the following settings:

- SA Rough
- Gauss Dist.
- Gauss Envel
- Correlation length / nm: 30000
- Gamma Layer / nm-2: Const 0,0026
- Height / nm: Const 97,7
- Period / nm: 900
- DutyCycle Base / %: 23,7
- Slope / %: 100
- In Plane Angle / deg: 83,3
- Divergence In Plane Angle / deg: 0,2
- Number of points per In Plane Angle: 5

This panel defines the height profile function describing the sample. Either by means of a predefined or a user defined height profile function.

The panel has three check boxes, *SA Rough*, *Gaussian Dist.* and *Gauss Envel*, and 9 input boxes.

SA Rough Check box

If checked the scattering is convoluted with the scattering determined by a Self-Affine roughness as defined by the *Isotropic Data panel*. The values taken for the Self-Affine roughness distribution are taken from that data.

Gauss Envelop check box

If checked the sample correlation function is multiplied by a Gaussian envelop function with a correlation length given by the input box Correlation length. This mimics a not perfect periodicity or represents an artificial resolution contribution. The formula used is

$$e^{-\frac{1}{2}\left(\frac{r}{r_c}\right)^2},$$

where r is the correlation distance and r_c the correlation length.

Gauss Dist. check box

If checked the sample is described by a height profile function. The correlation function is calculated assuming the grating is not perfect periodic, but has a Gaussian correlated distribution. The formula used depends on the selected approximation and is given in Appendix C. The height profile function can be predetermined or user defined. This is determined by the Grating data panel.

Correlation length input box

This value determines correlation length of the sample correlation function in nanometers. It is only enabled when the Gauss Envelop selection box is selected.

Gamma Layer input box

This value represents the scattering length density of the sample layer material times 4π in nanometer⁻² units.

Height Input box

This value determines the sample height in nanometers. If a height profile function is loaded it represents the total height of the loaded profile.

Period Input box

This value determines the sample repetition period in nanometers. If a height profile function is loaded it represents the repetition period of the loaded profile.

DutyCycle Base Input box

This value determines the sample base width of either block or trapezium in % of the period value.

Slope Input box

This value determines the slope in % of the trapezium. 100 % is an angle of 45 degrees. The minimum angle depends on the height of the sample, the period and the dutycycle of the base.

In Plane Angle Input box

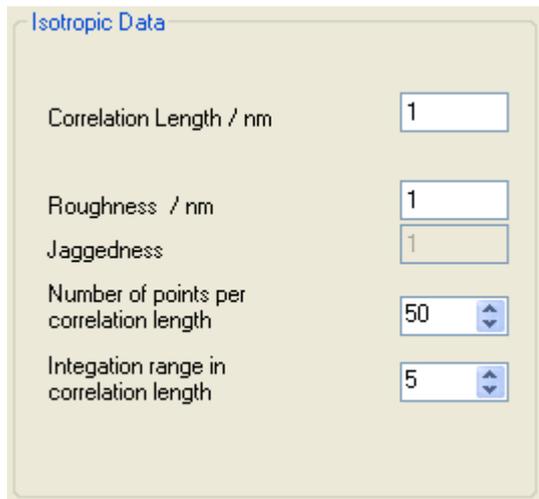
This value determines the orientation angle of the sample profile with respect to the beam. For 0° the grating profile is parallel to the beam direction and for 90° it is perpendicular.

Divergence In Plane Angle input box

This value determines the spread in the In Plane Angle parameter. The distribution function is a block with a constant width and amplitude given by this value.

Number of points per In Plane Angle input box

This number determines the number of interval steps used to calculate the influence of the divergence of the In Plane Angle parameter.

Isotropic Data panel


The screenshot shows a panel titled "Isotropic Data" with a light beige background. It contains five input fields arranged vertically on the left, each with a corresponding value in a box on the right:

- Correlation Length / nm: 1
- Roughness / nm: 1
- Jaggedness: 1
- Number of points per correlation length: 50 (with up and down arrow buttons)
- Integration range in correlation length: 5 (with up and down arrow buttons)

This panel defines the isotropic correlation functions describing the sample. Either by means of a predefined or by a user defined correlation function. It consists of 5 input boxes describing the correlation function, sample *Roughness*, *Correlation Length* and *Jaggedness*.

Correlation Length input box

This parameter defines the correlation length of the sample surface.

Roughness Input box

This parameter defines the Gaussian roughness of the sample surface.

Jaggedness input box (Only enabled for a Self-affine fractional correlation function)

This parameter defines the type of Gaussian roughness correlation function. A small value produces an extreme jagged surface and a value of 1 gives smooth hills and valleys. It is related to a fractal surface with fractal dimension $3 - Jaggedness$. See also the reference in footnote 3.

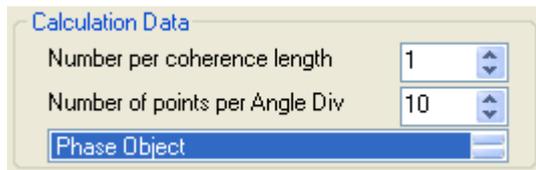
Number of points per correlation length input box

Determines the number of points used to calculate the correlation function. The larger the number, the *more accurate and slower* the calculations.

Integration range in correlation length input box

Determines the maximum range over which the correlation function extends in units of correlation lengths. The larger the range, the more accurate the results for small momentum transfer, and the less accurate the results for large momentum transfer. These can also be more accurate when the number of points per correlation length is increased. The larger the number, the *more accurate and slower* the calculations.

Calculation Data panel



This panel defines the theory used to perform the scattering calculations and some parameters needed to perform the calculations. The panel contains 2 input boxes and 3 selection boxes:

Number per Coherence length input box (for 1D profile)

This number determines the number of orders used to calculate the scattering for a periodic structure. (It corresponds to the range of n in the summations of Appendix C). In general, if the separate Q_x -cuts can be distinguished in the scattering, then this parameter can be 1. If they start to overlap, this number must be increased. If they coincide (due to scattering in the z -direction only), to get an accurate result the number must be taken large enough. A rule of thumb for an X-profile:

$$\begin{aligned} \text{Number of points Coherence length} &= \\ &= 1 + \text{Period} / \text{Coherence length} / \text{Cos (In Plane Angle)}, \end{aligned}$$

the Cos function changes into a Sin function for an Z-profile. It is wavelength dependent, as the coherence length is wavelength dependent. The calculations are *slower* if the number is *larger*.

Number per Coherence length input box (for 2D profile)

This number determines the number of intervals used to calculate the Fourier transform of the 2D correlation function determined from the user defined height profile function. The Fourier transform extends to 5 times the coherence length.

Number of points per Angle Div input box

This number determines the number of intervals used to calculate the influence of the width of the interval of the scattered angle channels.

Selection box

This selection enables the selection of the theory used for the calculations. Options are First Born approximation, Phase Object approximation, Distorted Wave Born approximation (see Appendix C for detail) or Extended Phase Object approximation (see Thanks Window, click on picture below text). The Extended Phase Object approximation is not implemented for the Gaussian distribution of the profile's. For this approximation one can either choose the height to be constant, or the scattering length density of the layer to be constant by selecting the appropriate radio button after the Height input box or Gamma Layer input box. For this approximation it is also possible to have a different scattering length density for the substrate and the layer. Note that the colour of the DWBA selection box turns *red* if the calculations render an unrealistic result, due to the imaginary part of the wave vector transfer becoming too

large negative. Then the criteria for the DWBA are not fulfilled. Roughly the criteria are: small disturbances (less than a few nanometer in height) only close to the critical edge, or far away from the critical edge.

Type selection box

With this box the type of data shown is selected. Chose Shim, Plus intensity, Min intensity or Polarization.

Calculate button

This button starts the calculations. It can take a while before it finishes. The bar directly to the right indicates progress made. During calculations the *Save button* changes into a *Stop button* that can be used for obvious reasons. *After stopping in this way, the data the calculated is not reliable!*

Save button

This button enables the data output. If pressed a file selection dialog will pop up requesting a filename. Extensions are OUT (for a space delimited file), OSV (for a TAB delimited file) or CSV (for a comma delimited file). If a valid filename is chosen the data will be saved under that name.

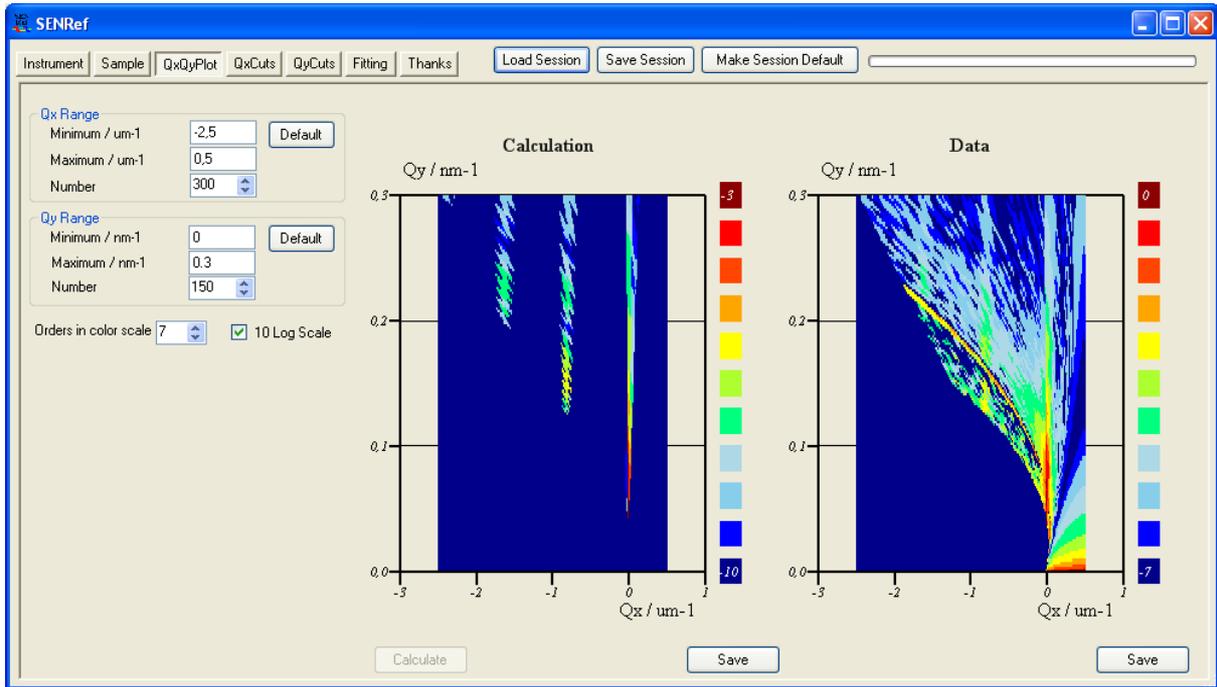
Orders in colour scale input box

The input box is a number to change the logarithmic colour scale of the graphs.

10 Log Scale selection box

If selected the output of the shown graph has a logarithmic scale.

6. QxQyPlot Window



The purpose of this window is for diagnostic purposes only. The data calculated matches the last calculation action performed on the Sample Window. The QxQy plot is calculated in such a way that the integral over Q_x , Q_y of the scattering function gives the same value as the integral over λ , α_p . To the left side this window has two panels: The Q_x Range panel and the Q_y Range panel. To the right side it has a selection box *10 Log Scale* and an input box *Orders in colour scale* and two output graphs showing the plots for the calculations and the data. At the bottom of the window three buttons appear: the *Calculate* button and two *Save* buttons.

Qx Range panel

Qx Range

Minimum / μm^{-1}

Maximum / μm^{-1}

Number

This panel consists of three input boxes: *Minimum*, *Maximum* and *Number* and a button *Default*. They define the linear range and step over which Q_x is varied. Note that the unit of Q_x is micrometer⁻¹. Pushing the default button changes the values to the range available in the calculations.

Qy Range panel

Qy Range

Minimum / nm^{-1}

Maximum / nm^{-1}

Number

This panel consists of three input boxes: *Minimum*, *Maximum* and *Number* and a button *Default*. They define the linear range and step over which Q_y is varied. Note that the unit of Q_y is nanometer^{-1} . Pushing the default button changes the values to the range available in the calculations.

Calculate button

This button starts the calculations. It can take a while before it finishes.

Save buttons

These button enable the data output. If pressed a file selection dialog will pop up requesting a filename. Extensions are OUT (for a space delimited file), OSV (for a TAB delimited file) or CSV (for a comma delimited file). If a valid filename is chosen the data will be saved under that name.

Orders in colour scale input box

The input box is a number to change the logarithmic colour scale of the graphs.

10 Log Scale selection box

If selected the output of the shown graph have a logarithmic scale.

7. QxCuts Window



The purpose of this window is for diagnostic purposes only. Be sure that the data calculated matches the required parameters (hence calculation is the last action performed on the Sample Window). To the left side this window has three panels: The *Qx Cuts Definition* panel, the *Qx cuts Generator* panel and the *Calculate Qx Cuts* panel. To the left bottom side it has a selection box *10 Log Scale* and an input box *Orders in log scale* and to the right an output graph showing the cuts. The cuts represent both the data (if available) as error bars and / or the calculations (if available) as lines. The corresponding Qx cuts have the same colour. The intensities are just the sum of all of the intensities in the points between the upper and lower limits of the Qx cut defined by $Qx\ max = Qx\ avg + Qx\ width$ and $Qx\ min = Qx\ avg - Qx\ width$. If Qx is equal to 0, the cut is the specular one between Incident Angle + Delta Angle and Incident Angle – Delta Angle. The Qx cut summation areas (if any are selected) will be shown as black lines on the graphs on the Sample Window and QxQyPlot Window.

Orders in colour scale input box

The input box is a number to change the logarithmic colour scale of the graphs.

10 Log Scale selection box

If selected the output of the shown graph have a logarithmic scale.

Qx Cuts Definition panel

The image shows two alternative configurations for the 'Qx Cuts Definition' panel. The left configuration has 'Number of cuts' set to 3, 'Selected cut' to 1, 'Qx avg / um-1' to -1,63, 'Qx width / um-1' to 0,0968, 'Min Wavelength / nm' to 0,101, and 'Max Wavelength / nm' to 0,991. The right configuration has 'Number of cuts' set to 3, 'Selected cut' to 3, 'Qx avg / um-1' to 0, 'Delta Angle /' to 1, 'Min Wavelength / nm' to 0,15, and 'Max Wavelength / nm' to 0,5. Both panels include an 'Enable Qx Cut' checkbox which is checked.

This panel defines the Qx cuts by means of 6 input boxes and 1 selection box:

Number of cuts input box

This number represents the number of cuts in the figure. Each Qx value is represented by one line in the graph.

Selected Cut input box

This number indicates from which Qx cut the values are indicated in the two lower input boxes.

Qx avg input box

This number gives the average Qx value of the cuts. When equal to 0 the lowest Input box of the current panel is changed to *Delta Angle* (unit milliradians), when different from 0 the lowest Input box is *Qx width* (unit micrometer⁻¹).

Delta Angle input box

This number determines the angle difference of the scattered angle between which the intensities are added to find the specular cut (unit milliradians).

Qx width input box

This number determines the intervals used to add the intensities for the specific Qx cut (unit micrometer⁻¹).

Min Wavelength input box

This number determines the minimum of the wavelength range used to calculate the cuts for the specific Qx cut.

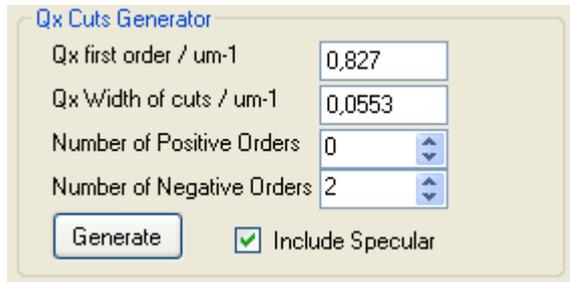
Max Wavelength input box

This number determines the maximum of the wavelength range used to calculate the cuts for the specific Qx cut.

Enable Qx Cut selection box

This indicates whether or not the selected cut should be plotted and fitted or not.

Qx Cuts Generator panel



The selection box, four input boxes and button on this panel can be used to generate the Qx cuts.

Qx first order input box

This number determines the Qx average value of the first order cut used to add the intensities for the specific Qx cut (unit micrometer⁻¹).

Qx width input box

This number determines the Qx interval width used to add the intensities for the specific Qx cut (unit micrometer⁻¹).

Number of Positive orders Input box

This number represents the number of Qx cuts with a positive order. All cuts for 1 to the indicated number are generated.

Number of Negative orders Input box

This number represents the number of Qx cuts with a negative order. All cuts for 1 to the indicated number are generated.

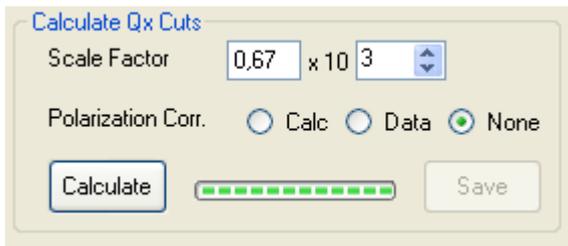
Include specular selection box

If the selection box is checked the generated Qx cuts will include the specular one. For the width of the specular one the resolution of the incident angle is taken (see Instrument Window, Instrument Panel, Resolution input box).

Generate button

Pressing this button generates the Qx cuts. The generated Qx cuts can be checked in the graph on the Sample Window and QxQyPlot window.

Calculate Qx Cuts panel



The input boxes and buttons on this panel can be used to (re-)calculate the Qx cuts and save them.

Scale Factor input boxes

This factor is used to change the scaling factor of the measurements. The calculations correspond to the number of neutrons or X-rays counted in the detector channel, except for a scaling factor. For comparison the scaling of the measurements can be adapted to match the one of the calculations.

Polarization Correction selection buttons

These buttons are visible if the polarization of the empty beam has been loaded using the *Load* button on the Instrument panel on the Instrument Window. If *Calc* is selected the calculated polarization is multiplied by the loaded empty beam polarization. If the wavelength is outside the available wavelength range, the calculated polarization is set to 0. If *Data* is selected the measured polarization is divided by the loaded empty beam polarization. If the wavelength is outside the available wavelength range, the measured polarization is set to 0. If *None* is selected no correction is done. Remember to use the *Calculate* button to let the changed selection take effect.

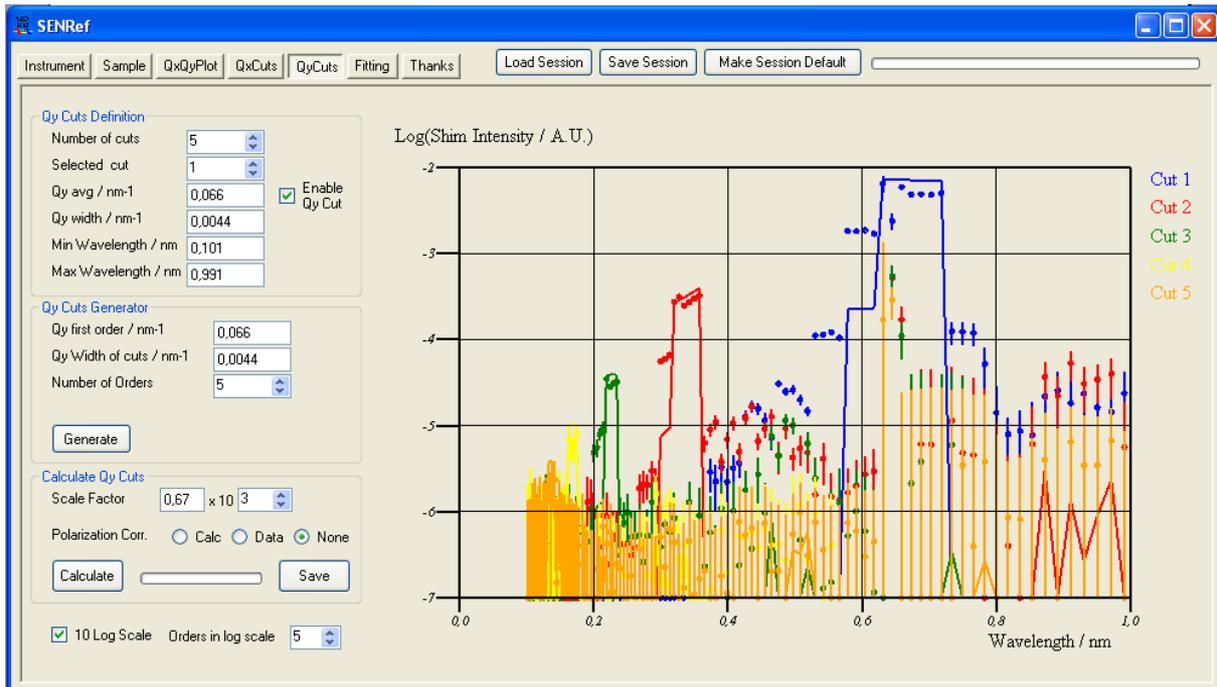
Calculate button

Pressing this button (re-)calculates the Qx cuts. The Qx cuts can be checked in the graph to the right.

Save button

This button enables the data output. If pressed a file selection dialog will pop up requesting a filename. Extensions are OUT (for a space delimited file), OSV (for a TAB delimited file) or CSV (for a comma delimited file). If a valid filename is chosen the data will be saved under that name.

8. QyCuts Window



The purpose of this window is for diagnostic purposes only. Be sure that the data calculated matches the required parameters (hence calculation is the last action performed on the Sample Window). To the left side this window has three panels: The *Qy Cuts Definition* panel, the *Qy cuts Generator* panel and the *Calculate Qy Cuts* panel. At the left bottom side it has a selection box *10 Log Scale* and an input box *Orders in log scale* and to the right an output graph showing the cuts. The cuts represent both the data (if available) as error bars and / or the calculations (if available) as lines. The corresponding Qy cuts have the same colour. The intensities are just the sum of all of the intensities of the points between the upper and lower limits of the Qy cut, defined by $Qy\ max = Qy\ avg + Qy\ width$ and $Qy\ min = Qy\ avg - Qy\ width$. The Qy cut summation areas (if any are selected) will be shown as black lines on the graphs on the Sample Window and QxQyPlot Window.

Orders in colour scale input box

The input box is a number to change the logarithmic colour scale of the graphs.

10 Log Scale selection box

If selected the output of the shown graph have a logarithmic scale.

Qy Cuts Definition panel

The screenshot shows a panel titled "Qy Cuts Definition" with the following fields and values:

Number of cuts	5	
Selected cut	1	
Qy avg / nm-1	0,066	<input checked="" type="checkbox"/> Enable Qy Cut
Qy width / nm-1	0,0044	
Min Wavelength / nm	0,101	
Max Wavelength / nm	0,991	

This panel defines the Qy cuts by means of 6 input boxes and 1 selection box:

Number of cuts input box

This number represents the number of cuts in the figure. Each Qy value is represented by one line in the graph.

Selected Cut input box

This number indicates from which Qy cut the values are indicated in the two lower input boxes.

Qy avg input box

This number determines the value of the average Qy value the cuts should (unit nanometer-1).

Qy width input box

This number determines the intervals used to add the intensities for the specific Qy cut (unit nanometer-1).

Min Wavelength input box

This number determines the minimum of the wavelength range used to calculate the cuts for the specific Qy cut.

Max Wavelength input box

This number determines the maximum of the wavelength range used to calculate the cuts for the specific Qy cut.

Enable Qy Cut selection box

This indicates whether or not the selected cut should be plotted and fitted or not.

Qy Cuts Generator panel

The three input boxes and button on this panel can be used to generate the Qy cuts.

Qy first order input box

This number determines the Qy average value used for the specific Qy cut (unit nanometer-1). Default value is determined by the height of the sample.

Qy width input box

This number determines the Qy interval width used to add the intensities for the specific Qy cut (unit nanometer-1). Default value is determined by the height of the sample.

Number of orders input box

This number represents the number of Qy cuts. All cuts for 1 to the indicated number are generated.

Generate button

Pressing this button generates the Qy cuts. The generated Qy cuts can be checked in the graph on the Sample Window and QxQyPlot window.

Calculate Qy Cuts panel

The input boxes and buttons on this panel can be used to (re-)calculate the Qy cuts and save them:

Scale Factor input boxes

This factor is used to change the scaling factor of the measurements. The calculations correspond to the number of neutrons or X-rays counted in the detector channel, except for a scaling factor. For comparison the scaling of the measurements can be adapted to match the one of the calculations.

Polarization Correction selection buttons

These buttons are visible if the polarization of the empty beam has been loaded using the *Load* button on the Instrument panel on the Instrument Window. If *Calc* is selected the calculated polarization is multiplied by the loaded empty beam polarization. If the wavelength is outside the available wavelength range, the calculated polarization is set to 0. If *Data* is selected the measured polarization is divided by the loaded empty beam polarization. If the wavelength is outside the available wavelength range, the measured polarization is set to 0. If *None* is selected no correction is done. Remember to use the *Calculate button* to let the changed selection take effect.

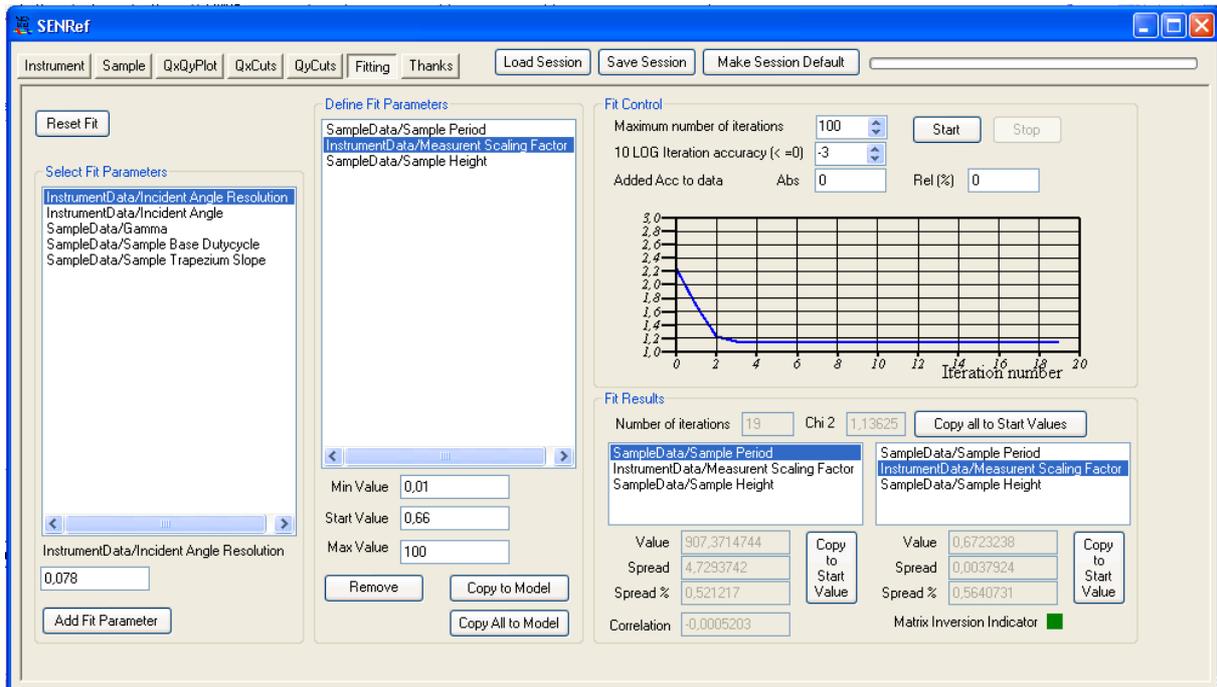
Calculate button

Pressing this button (re-)calculates the Qy cuts. The Qy cuts can be checked in the graph to the right.

Save button

This button enables the data output. If pressed a file selection dialog will pop up requesting a filename. Extensions are OUT (for a space delimited file), OSV (for a TAB delimited file) or CSV (for a comma delimited file). If a valid filename is chosen the data will be saved under that name.

9. Fitting Window



The purpose of this window is for fitting the model to the data. The data fitted are the cuts defined and enabled on the QxCuts and QyCuts Windows. The program only calculated the point needed to determine these cuts. Lesser cuts and the smaller ranges increase the fit speed. The fit is based on the minimization of the so called chi-squared, i.e. The average quadrate of the difference between fit and data point divided by the error. The minimization procedure is based on the Marquardt-Levenberg method. This method calculates the steepest decent from the matrix inversion of the Jacobian matrix. If a change in a fit parameter has no influence (or very small) on the calculated chi-squared, the possibility exist that the inversion of the Jacobian matrix is singular and the fit does not converge to the (local) minimum. This is indicated by the Matrix inversion indicator turning to red. The window has three control panels, *Select Fit Parameters*, *Define Fit Parameters* and *Fit Control* and a results panel, *Fit Results* and a button, *Reset Fit*.

Reset Fit button

Pressing this button initialized the model parameters. The start values are taken from the Instrument and Sample Windows.

Select Fit Parameters panel



The selection box, input box and button on this panel can be used to select the fit parameter.

Selection box

The selection box shows all possible parameters which can be fitted for the instrument and sample model chosen. Selecting a parameter will change the value of the input box under the selection box. The name of the parameter will appear in the output box.

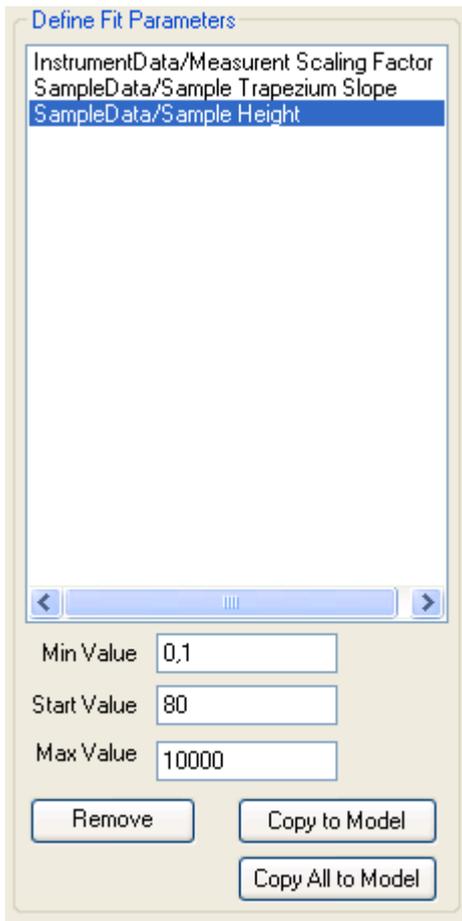
Input box

This value is the initial value of the selected fit parameter.

Add Fit Parameter button

If this button is pressed the parameter is removed from the above mentioned selection box and moved to the selection box in the Define Fit Parameters panel. This parameter will now be fitted.

Define Fit Parameters panel



The selection box, three input boxes and three buttons on this panel can be used to set the right upper and lower limits of the fit parameters. The smaller the range the faster and reliable the algorithm will find the desired minimum.

Selection box

The selection box shows all parameters are fitted. Selecting a parameter will change the value of the input boxes under the selection box.

Min Value input box

This value determines the lower limit of the fit parameter selected in the selection box.

Start Value input box

This value determines the initial value of the fit parameter selected in the selection box.

Max Value input box

This value determines the upper limit of the fit parameter selected in the selection box.

Remove button

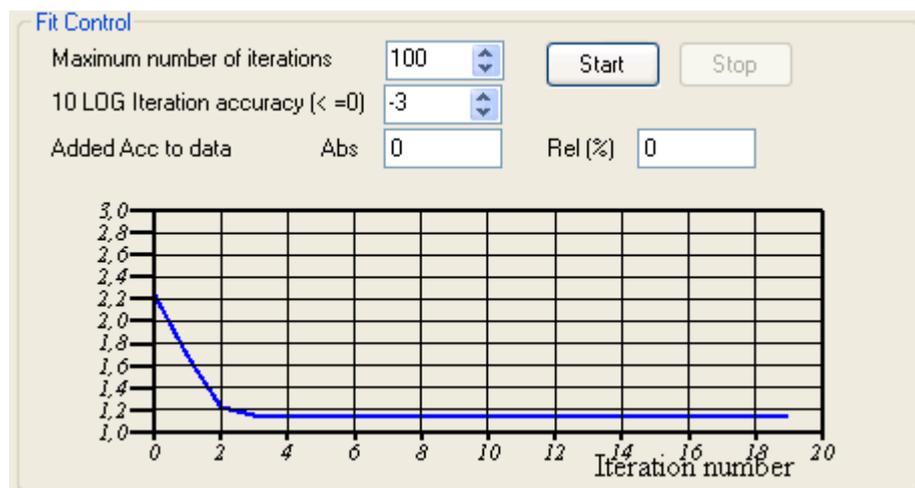
If this button is pressed the parameter is removed from the above mentioned selection box and returned to the selection box in the Select Fit Parameters panel. This parameter will **is not** fitted anymore.

Copy to model button

If this button is pressed the actual value of the parameter selected in the above selection box is copied to the parameter in the Instrument or Sample Window. The previous value of this parameters is lost.

Copy All to model button

If this button is pressed the actual value of all possible fit parameters in the both selection boxes of the Select and Define Fit Parameter Panels are copied to the respective parameters in the Instrument or Sample Window. The previous values of these parameters are lost.

Control Fit panel

The four input boxes and two buttons on this panel can be used to control the fitting procedure. The graph at the lower side of the panel shows the chi-squared as function of the iteration number.

Maximum number of iterations input box

This number determines the maximum number of iterations. The fit can stop sooner, if the required accuracy in chi-squared is reached.

10 LOG Iteration accuracy input box

This number determines fit accuracy. It is used as a measure of the step size to determine the gradient of the function and it determines the minimum change in chi-squared to continue fitting.

Abs input box

This value is added to the error of each cut point value to manipulate the fitting. For instance, it can be used to overcome faulty error bars due to wrong background subtraction.

Rel(%) input box

This value is the percentage of the cut point value that is added to the error of each cut point value to manipulate the fitting. For instance, it can be used to overcome faulty error bars due to wrong scaling.

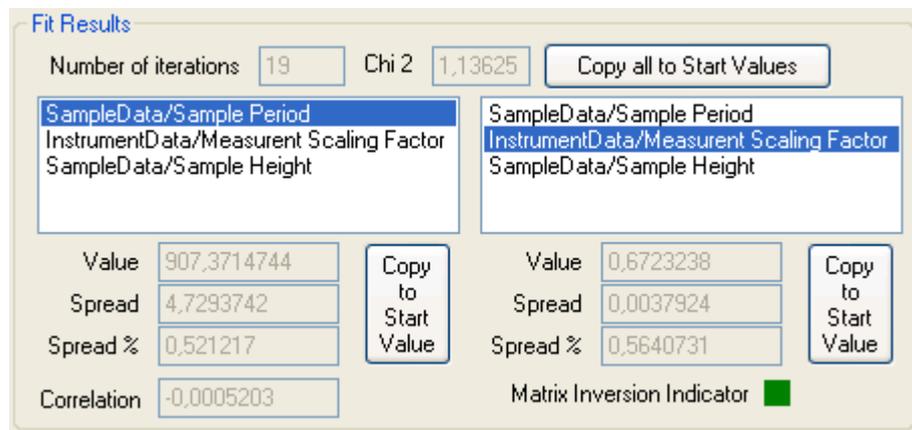
Start button

Enables the start of the fit procedure. All input boxes or buttons on all windows are disabled. It is possible to change to another Window during the fit to investigate its progress on either the Sample, QxCuts or QyCuts Windows.

Stop button

If pressed the fit is stopped after the current iteration is finished. The start button can be pressed again and de fit will restart.

Fit Results panel



The two selection boxes and three buttons on this panel can be used to investigate the fit results and copy the values to the initial fit values. The output boxes show information on the fit parameters selected in the selection boxes above. The *Spread output boxes* are calculated using the co-variance matrix determined from the Jacobian matrix. It is an indication of the accuracy of the selected fit parameter. The *Correlation output box* is the correlation between the selected fit parameters.

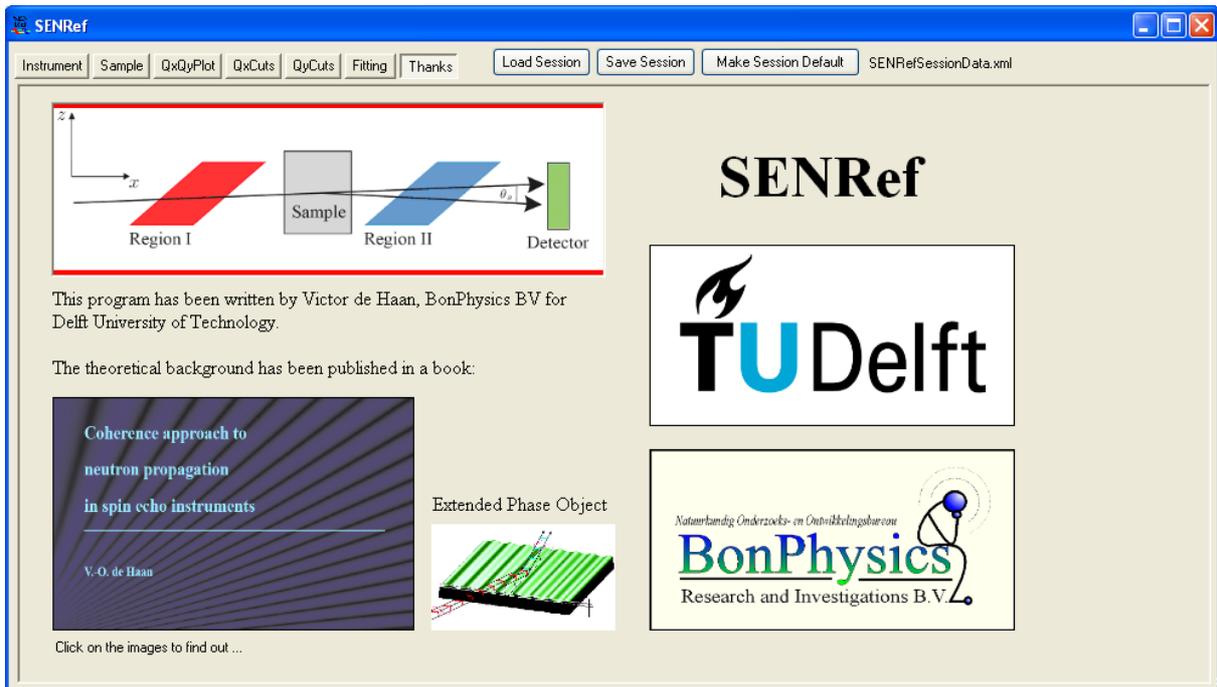
Copy to Start Value button

If pressed the actual value of the selected fit parameter is copied to its initial value. This enables the continuation of the fit with the end value of the previous fit.

Copy All to Start Value button

If pressed the actual value of all fit parameters are copied to their initial value. This enables the continuation of the previous fit.

10. Thanks Window



The purpose of this window is for information purposes only. You can find this guide by clicking on the upper left picture. The theoretical background for the calculations can be found in the book 'Coherence approach to neutron propagation in spin echo instruments'. This is opened if the lower left picture is clicked. Clicking on the Extended Phase Object gives information about these calculations. Clicking the right pictures opens the home pages of the corresponding institutes.

Appendix A: Format of Data file

The files are simple ASCII files. The input format is as follows:

Up Spin *or* Down Spin *or* Non-Polarized

Without Errors:

[Y0 Y1 Y2 Yn Yn+1//

X1 D11 D12 D1n//

X2 D21 D22 D2n//

...

Xm Dm1 Dm2 Dmn//

Xm+1]

Up Spin *or* Down Spin *or* Non-Polarized

With Errors:

[Y0 Y1 Y1 Y2 Y2 Yn Yn Yn+1 Yn+1//

X1 D11 E11 D12 E12 D1n E1n//

X2 D21 E21 D22 E22 D2n E2n//

.....

Xm Dm1 Em1 Dm2 Em2 Dmn Emn//

Xm+1]

Polarized

Without Errors:

[Y0 Y1 Y1 Y2 Y2 Yn Yn Yn+1 Yn+1//

X1 P11 M11 P12 M12 P1n M1n//

X1 P21 M21 P22 M22 P2n M2n//

.....

Xm Pm1 Mm1 Pm2 Mm2 P1m M1m//

Xm+1]

Polarized

With Errors:

```
[Y0 Y1 Y1 Y1 Y1 Y2 Y2 Y2 Y2 ..... Yn Yn Yn Yn Yn+1 Yn+1//
X1 P11 EP11 M11 EM11 P12 EP12 M12 EM12 ..... P1n EP1n M1n EM1n//
X2 P21 EP21 M21 EM21 P22 EP22 M22 EM22 ..... P2n EP2n M2n EM2n//
.....
Xm Pm1 EPm1 Mm1 EMm1 Pm2 EPm2 Mm2 EMm2 ..... Pmn EPmn Mmn EMmn//
Xm+1]
```

Where:

‘ [‘ indicates start of file

‘ //‘ indicates end of line

‘]’ indicates end of file

‘ ’ indicates user required repetition of sequence

Y0 is a number: Not used

Yi (i=1..n) : start values of scattered angle interval i (In ascending order)

Yi+1 (i=1..n) : end values of scattered angle interval i (In ascending order)

Xj (j=1..m): start value of incident angle (Monochromatic mode) or wavelength (TOF-mode) interval j (In ascending order)

Xj+1 (j=1..m): end value of incident angle (Monochromatic mode) or wavelength (TOF-mode) interval j (In ascending order)

Dij: Data values for Xj;Yi

Eij: Error in data values for Xj;Yi (standard deviation)

Pij: Data values Up Spin for Xj;Yi

EPij: Error in data values Up Spin for Xj;Yi (standard deviation)

Mij: Data values Down Spin for Xj;Yi

EMij: Error in data values Down Spin for Xj;Yi (standard deviation)

Appendix B: Format of Data file

(1 Dimensional Profile and Empty beam polarization)

The files are simple ASCII files. The input format is as follows:

```
[Y0 Y1//  
X1 D1//  
X2 D2//  
...  
Xm Dm]
```

Where:

‘ [‘ indicates start of file

‘ //‘ indicates end of line

‘]’ indicates end of file

‘’ indicates user required repetition of sequence

Y0 is a number: Not used

Y1 is a number: Not used

Xj (j=1..m): Distance (Profile mode) or wavelength (Polarization mode) in [nm]

Dj: Data values for Xj: Height in [nm] (Profile mode) or Polarization

Appendix C: Background of performed calculations.

In general the calculations are done using the equations described in chapter 6 of the reference of footnote 2. To speed up the calculations it was assumed that the incident mutual coherence function on the sample position was homogeneous and Gaussian distributed with a large coherence length in the beam direction and a small one in the direction perpendicular to it. The coherence length is the standard deviation of the Gaussian distribution.

In principle the spin-echo signal for a grating must be determined using eqs. (7.14) and (7.15) of reference in footnote 2. However, if there is only structure in the z -direction and the in plane angle is 0, then eq. (7.24) can be used to speed up the calculations. If some in-plane angle different from 0 is used in principle this is wrong, for the scattering in the x -direction. Then the *Number per Coherence length* parameter must be increased to find the correct spin-echo signal for the scattering.

In the following the basic equations for the several sample types and approximations are given.

DWBA *General*

Sample surface correlation function

(Combination of eqs. (6.96) to (6.99) of reference in footnote 2):

$$G_s^{(0,0)}(\vec{p}) = A_s R(p_y) \frac{p_y^2}{4\pi^2} = A_s \left(\frac{\Gamma T(p_y)}{8\pi p_y} \right)^2$$

$$G_s^{Spec}(\vec{p}, \vec{k}, \vec{r}_{||}) = G_s^{(0,0)}(\vec{p}) \left| 1 + \frac{p_y}{p'_y} E \left(e^{-2ip'_y H(\vec{r}_s)} - 1 \right) \right|^2$$

$$G_s^{OffSpec}(\vec{p}, \vec{k}, \vec{r}_{||}) = G_s^{(0,0)}(\vec{p}) \frac{4p_y^2}{|\kappa_y|^2} \frac{T(k_y)}{T(p_y)} \left(E \left(e^{i(\kappa_y)^* H(\vec{r}_{||} + \vec{r}_s) - i\kappa_y H(\vec{r}_s)} \right) - \left| E \left(e^{-i\kappa_y H(\vec{r}_s)} \right) \right|^2 \right)$$

Sample surface scattering function

(Combination of eqs. (6.104) to (6.107) of reference in footnote 2):

$$S_k(\vec{p}, \vec{k}) = \int e^{-i\vec{Q}_{||}\vec{r}_{||}} G_s(\vec{p}, \vec{k}, \vec{r}_{||}) d^2 r_{||}$$

$$S_k(\vec{p}, \vec{k}) = S_k^{Spec}(\vec{p}, \vec{k}) + S_k^{OffSpec}(\vec{p}, \vec{k})$$

$$S_k^{Spec}(\vec{p}, \vec{k}) = 4\pi^2 A_s \left(\frac{\Gamma T(p_y)}{8\pi p_y} \right)^2 \delta^2(\vec{Q}_{||}) \left| 1 + \frac{p_y}{p'_y} E \left(e^{-2ip'_y H(\vec{r}_s)} - 1 \right) \right|^2$$

$$S_k^{OffSpec}(\vec{p}, \vec{k}) = A_s \Gamma^2 \frac{T(p_y) T(k_y)}{16\pi^2 |\kappa_y|^2} \left\{ \int e^{-i\vec{Q}_{||}\vec{r}_{||}} E \left(e^{i(\kappa_y)^* H(\vec{r}_{||} + \vec{r}_s) - i\kappa_y H(\vec{r}_s)} \right) d^2 r_{||} - 4\pi^2 \delta^2(\vec{Q}_{||}) \left| E \left(e^{-i\kappa_y H(\vec{r}_s)} \right) \right|^2 \right\}$$

or

$$S_k^{OffSpec}(\vec{p}, \vec{k}) = A_s \Gamma^2 \frac{T(p_y) T(k_y)}{16\pi^2 |\kappa_y|^2} \left\{ \left| \int e^{-i\vec{Q}_{||}\vec{r}_{||}} e^{-i\kappa_y H(\vec{r}_{||})} d^2 r_{||} \right|^2 - 4\pi^2 \delta^2(\vec{Q}_{||}) \left| E \left(e^{-i\kappa_y H(\vec{r}_s)} \right) \right|^2 \right\}$$

DWBA *Gaussian Random Distribution*

(standard deviation σ , average μ , complex constant q):

$$E\left(e^{iqH(\vec{r}_s)}\right) = e^{-\sigma^2 q^2 / 2 + i\mu q}$$

$$E\left(e^{i(\kappa_y)^* H(\vec{r}_\parallel + \vec{r}_s) - i\kappa_y H(\vec{r}_s)}\right) = e^{-|\kappa_y|^2 (\sigma^2 - C(\vec{r}_\parallel))} e^{-\left(\kappa_y - (\kappa_y)^*\right)^2 \sigma^2 / 2}$$

$$C(\vec{r}_\parallel) = \frac{1}{A_s} \int_{A_s} H(\vec{r}_s) H(\vec{r}_s + \vec{r}_\parallel) d^2 r_s, \quad C(0) = \sigma^2$$

Sample surface correlation function:

$$G_s^{Spec}(\vec{p}, \vec{k}, \vec{r}_\parallel) = G_s^{(0,0)}(\vec{p}) \left| 1 + \frac{p_y}{p'_y} \left(e^{-2p_y^2 \sigma^2} - 1 \right) \right|^2$$

$$G_s^{OffSpec}(\vec{p}, \vec{k}, \vec{r}_\parallel) = G_s^{(0,0)}(\vec{p}) \frac{4p_y^2 T(k_y)}{|\kappa_y|^2 T(p_y)} e^{-\text{Re}\{\kappa_y^2\} \sigma^2} \left(e^{|\kappa_y|^2 C(\vec{r}_\parallel)} - 1 \right)$$

Sample surface scattering function:

$$S_k^{Spec}(\vec{p}, \vec{k}) = 4\pi^2 A_s \left(\frac{\Gamma T(p_y)}{8\pi p_y} \right)^2 \delta^2(\vec{Q}_\parallel) \left| 1 + \frac{p_y}{p'_y} \left(e^{-2p_y^2 \sigma^2} - 1 \right) \right|^2$$

$$S_k^{OffSpec}(\vec{p}, \vec{k}) = A_s \Gamma^2 \frac{T(p_y) T(k_y)}{16\pi^2 |\kappa_y|^2} e^{-\text{Re}\{\kappa_y^2\} \sigma^2} \int e^{-i\vec{Q}_\parallel \vec{r}_\parallel} \left(e^{|\kappa_y|^2 C(\vec{r}_\parallel)} - 1 \right) d^2 r_\parallel$$

DWBA *Block*

(Height H , Period L , Width D)

$$E\left(e^{iqH(x_s)}\right) = 1 + \frac{D}{L}\left(e^{iqH} - 1\right)$$

$$0 \leq x < D \quad E\left(e^{i(\kappa_y)^* H(x+x_s) - i\kappa_y H(x_s)}\right) = 1 - \frac{D}{L}\left(1 - e^{-2H\text{Im}\{\kappa_y\}}\right) + \frac{x}{L}\left(2e^{-H\text{Im}\{\kappa_y\}} \cos\left(H \text{Re}\{\kappa_y\}\right) - 1 - e^{-2H\text{Im}\{\kappa_y\}}\right)$$

$$D \leq x < \frac{L}{2} \quad E\left(e^{i(\kappa_y)^* H(x+x_s) - i\kappa_y H(x_s)}\right) = 1 + \frac{2D}{L}\left(e^{-H\text{Im}\{\kappa_y\}} \cos\left(H \text{Re}\{\kappa_y\}\right) - 1\right)$$

Sample surface correlation function:

$$G_s^{Spec}\left(\vec{p}, \vec{k}, \vec{r}_{//}\right) = G_s^{(0,0)}\left(\vec{p}\right) \left| 1 + \frac{D}{L} \frac{p_y}{p'_y} \left(e^{-2ip'_y H} - 1\right) \right|^2$$

$$0 \leq x < D \quad G_s^{OffSpec}\left(\vec{p}, \vec{k}, \vec{r}_{//}\right) = G_s^{(0,0)}\left(\vec{p}\right) \frac{4p_y^2}{|\kappa_y|^2} \frac{T(k_y)}{T(p_y)} \left(\frac{x}{L} - \frac{D}{L} + \left(\frac{D}{L}\right)^2\right) \left(2e^{-H\text{Im}\{\kappa_y\}} \cos\left(H \text{Re}\{\kappa_y\}\right) - 1 - e^{-2H\text{Im}\{\kappa_y\}}\right)$$

$$D \leq x < \frac{L}{2} \quad G_s^{OffSpec}\left(\vec{p}, \vec{k}, \vec{r}_{//}\right) = G_s^{(0,0)}\left(\vec{p}\right) \frac{4p_y^2}{|\kappa_y|^2} \frac{T(k_y)}{T(p_y)} \left(\frac{D}{L}\right)^2 \left(2e^{-H\text{Im}\{\kappa_y\}} \cos\left(H \text{Re}\{\kappa_y\}\right) - 1 - e^{-2H\text{Im}\{\kappa_y\}}\right)$$

Sample surface scattering function:

$$S_k^{Spec}\left(\vec{p}, \vec{k}\right) = 4\pi^2 A_s \left(\frac{\Gamma T(p_y)}{8\pi p_y}\right)^2 \delta^2\left(\vec{Q}_{//}\right) \left| 1 + \frac{D}{L} \frac{p_y}{p'_y} \left(e^{-2ip'_y H} - 1\right) \right|^2$$

$$S_k^{OffSpec}\left(\vec{p}, \vec{k}\right) = A_s \Gamma^2 \frac{T(p_y) T(k_y)}{4|\kappa_y|^2} \delta(Q_z) \left(e^{-2H\text{Im}\{\kappa_y\}} - 2e^{-H\text{Im}\{\kappa_y\}} \cos\left(H \text{Re}\{\kappa_y\}\right) + 1\right) \times \\ \times \sum_{n=-\infty, n \neq 0}^{\infty} \delta(Q_x - 2n\pi) \frac{\sin^2\left(n\pi \frac{D}{L}\right)}{(n\pi)^2}$$

DWBA *Block Gaussian Distributed*

(Height H , Period L , Width D)

$$E\left(e^{iqH(\bar{r}_s)}\right) = e^{-\sigma^2 q^2 / 2 + i\mu q}$$

$$E\left(e^{i(\kappa_y)^* H(\bar{r}_j + \bar{r}_s) - i\kappa_y H(\bar{r}_s)}\right) = e^{-|\kappa_y|^2 (\sigma^2 - C(\bar{r}_j))} e^{-(\kappa_y - (\kappa_y)^*)^2 \sigma^2 / 2}$$

$$0 \leq x < D \quad C(\bar{r}_j) = H^2 \left(\frac{D-x}{L} - \left(\frac{D}{L} \right)^2 \right)$$

$$D \leq x < \frac{L}{2} \quad C(\bar{r}_j) = -H^2 \left(\frac{D}{L} \right)^2$$

$$C(0) = \sigma^2 = H^2 \frac{D}{L} \left(1 - \frac{D}{L} \right)$$

Sample surface correlation function:

$$G_s^{Spec}(\bar{p}, \bar{k}, \bar{r}_j) = G_s^{(0,0)}(\bar{p}) \left| 1 + \frac{p_y}{p'_y} \left(e^{-2p_y^2 \sigma^2} - 1 \right) \right|^2$$

$$G_s^{OffSpec}(\bar{p}, \bar{k}, \bar{r}_j) = G_s^{(0,0)}(\bar{p}) \frac{4p_y^2}{|\kappa_y|^2} \frac{T(k_y)}{T(p_y)} e^{-\text{Re}\{\kappa_y^2\} \sigma^2} \left(e^{|\kappa_y|^2 C(\bar{r}_j)} - 1 \right)$$

$$0 \leq x < D \quad G_s^{OffSpec}(\bar{p}, \bar{k}, \bar{r}_j) = G_s^{(0,0)}(\bar{p}) \frac{4p_y^2}{|\kappa_y|^2} \frac{T(k_y)}{T(p_y)} e^{-\text{Re}\{\kappa_y^2\} \sigma^2} \left(e^{H^2 |\kappa_y|^2 \left(\frac{D-x}{L} - \left(\frac{D}{L} \right)^2 \right)} - 1 \right)$$

$$D \leq x < \frac{L}{2} \quad G_s^{OffSpec}(\bar{p}, \bar{k}, \bar{r}_j) = G_s^{(0,0)}(\bar{p}) \frac{4p_y^2}{|\kappa_y|^2} \frac{T(k_y)}{T(p_y)} e^{-\text{Re}\{\kappa_y^2\} \sigma^2} \left(e^{-|\kappa_y|^2 H^2 \left(\frac{D}{L} \right)^2} - 1 \right)$$

Sample surface scattering function:

$$S_k^{Spec}(\bar{p}, \bar{k}) = 4\pi^2 A_s \left(\frac{\Gamma T(p_y)}{8\pi p_y} \right)^2 \delta^2(\bar{Q}_j) \left| 1 + \frac{p_y}{p'_y} \left(e^{-2p_y^2 \sigma^2} - 1 \right) \right|^2$$

$$S_k^{OffSpec}(\bar{p}, \bar{k}) = A_s \Gamma^2 \frac{T(p_y) T(k_y)}{4|\kappa_y|^2} e^{2\text{Im}\{\kappa_y\} \sigma^2} \delta(Q_z) \times$$

$$\times \sum_{n=-\infty, n \neq 0}^{\infty} \frac{H^2 |\kappa_y|^2 \delta\left(Q_x - \frac{2n\pi}{L}\right)}{\left(H^2 |\kappa_y|^2\right)^2 + (2n\pi)^2} \left[1 - \left(H^2 |\kappa_y|^2 \frac{\sin\left(2n\pi \frac{D}{L}\right)}{2n\pi} + \cos\left(2n\pi \frac{D}{L}\right) \right) e^{-\frac{D}{L} H^2 |\kappa_y|^2} \right]$$

Phase-Object *General*

Sample surface correlation function

(Fourier transform of eq. (6.124) of reference in footnote 2):

$$R_{PO}(k_y, p_y) = \left| \frac{p_y - p'_y}{k_y - p'_y} \right|^2$$

$$G_s^{(0,0)}(\vec{k}) = A_s R_{PO}(-p_y, p_y) \frac{p_y^2}{4\pi^2}$$

$$G_s^{Spec}(\vec{p}, \vec{k}, \vec{r}_\parallel) = G_s^{(0,0)}(\vec{k}) \left| E(e^{-iq_y H(\vec{r}_s)}) \right|^2$$

$$G_s^{OffSpec}(\vec{p}, \vec{k}, \vec{r}_\parallel) = G_s^{(0,0)}(\vec{k}) \frac{R_{PO}(k_y, p_y)}{R_{PO}(-p_y, p_y)} \left(E(e^{iq_y (H(\vec{r}_\parallel + \vec{r}_s) - H(\vec{r}_s))}) - \left| E(e^{-iq_y H(\vec{r}_s)}) \right|^2 \right)$$

Sample surface scattering function (eq. (6.124) of reference in footnote 2):

$$S_k^{Spec}(\vec{p}, \vec{k}) = A_s R_{PO}(-p_y, p_y) p_y^2 \delta^2(\vec{Q}_\parallel) \left| E(e^{-iq_y H(\vec{r}_s)}) \right|^2$$

$$S_k^{OffSpec}(\vec{p}, \vec{k}) = A_s R_{PO}(k_y, p_y) \frac{p_y^2}{4\pi^2} \left\{ \int e^{-i\vec{Q}_\parallel \vec{r}_\parallel} E(e^{iq_y (H(\vec{r}_\parallel + \vec{r}_s) - H(\vec{r}_s))}) d^2 r_\parallel - 4\pi^2 \delta^2(\vec{Q}_\parallel) \left| E(e^{-iq_y H(\vec{r}_s)}) \right|^2 \right\}$$

or

$$S_k^{OffSpec}(\vec{p}, \vec{k}) = A_s R_{PO}(k_y, p_y) \frac{p_y^2}{4\pi^2} \left\{ \left| \int e^{-i\vec{Q}_\parallel \vec{r}_\parallel} e^{-iq_y H(\vec{r}_\parallel)} d^2 r_\parallel \right|^2 - 4\pi^2 \delta^2(\vec{Q}_\parallel) \left| E(e^{-iq_y H(\vec{r}_s)}) \right|^2 \right\}$$

Phase-Object *Gaussian Random Distribution*

(standard deviation σ , average μ , complex constant q):

$$E\left(e^{iqH(\vec{r}_s)}\right) = e^{-\sigma^2 q^2 / 2 + i\mu q}$$

$$E\left(e^{iq_y(H(\vec{r}_s + \vec{r}_s) - H(\vec{r}_s))}\right) = e^{-q_y^2(\sigma^2 - C(\vec{r}_s))}$$

$$C(\vec{r}_s) = \frac{1}{A_s} \int_{A_s} H(\vec{r}_s) H(\vec{r}_s + \vec{r}_s) d^2 r_s, \quad C(0) = \sigma^2$$

Sample surface correlation function:

$$G_s^{Spec}(\vec{p}, \vec{k}, \vec{r}_s) = G_s^{(0,0)}(\vec{k}) e^{-\sigma^2 q_y^2}$$

$$G_s^{OffSpec}(\vec{p}, \vec{k}, \vec{r}_s) = G_s^{(0,0)}(\vec{k}) \frac{R_{PO}(k_y, p_y)}{R_{PO}(-p_y, p_y)} e^{-\sigma^2 q_y^2} \left(e^{q_y^2 C(\vec{r}_s)} - 1 \right)$$

Sample surface scattering function:

$$S_k^{Spec}(\vec{p}, \vec{k}) = \delta^2(\vec{Q}_s) A_s R_{PO}(-p_y, p_y) p_y^2 e^{-\sigma^2 q_y^2}$$

$$S_k^{OffSpec}(\vec{p}, \vec{k}) = A_s R_{PO}(k_y, p_y) p_y^2 e^{-\sigma^2 q_y^2} \int e^{-i\vec{Q}_s \cdot \vec{r}_s} \left(e^{q_y^2 C(\vec{r}_s)} - 1 \right) d^2 r_s$$

Phase-Object *Block*

(Height H , Period L , Width D)

$$E\left(e^{iqH(x_s)}\right) = 1 + \frac{D}{L}\left(e^{iqH} - 1\right)$$

$$0 \leq x < D \quad E\left(e^{iq_y(H(x+x_s)-H(x_s))}\right) = 1 + \frac{2x}{L}\left(\cos(q_y H) - 1\right)$$

$$D \leq x < \frac{L}{2} \quad E\left(e^{iq_y(H(x+x_s)-H(x_s))}\right) = 1 + \frac{2D}{L}\left(\cos(q_y H) - 1\right)$$

Sample surface correlation function:

$$G_s^{Spec}(\vec{p}, \vec{k}, \vec{r}_{//}) = G_s^{(0,0)}(\vec{k}) \left(1 - 2\frac{D}{L}\left(1 - \frac{D}{L}\right)(1 - \cos(q_y H))\right)$$

$$0 \leq x < D \quad G_s^{OffSpec}(\vec{p}, \vec{k}, \vec{r}_{//}) = G_s^{(0,0)}(\vec{k}) \frac{R_{PO}(k_y, p_y)}{R_{PO}(-p_y, p_y)} 2(\cos(q_y H) - 1) \left(\frac{x}{L} - \frac{D}{L} + \left(\frac{D}{L}\right)^2\right)$$

$$D \leq x < \frac{L}{2} \quad G_s^{OffSpec}(\vec{p}, \vec{k}, \vec{r}_{//}) = G_s^{(0,0)}(\vec{k}) \frac{R_{PO}(k_y, p_y)}{R_{PO}(-p_y, p_y)} 2(\cos(q_y H) - 1) \left(\frac{D}{L}\right)^2$$

Sample surface scattering function:

$$S_k^{Spec}(\vec{p}, \vec{k}) = \delta^2(\vec{Q}_{//}) A_s R_{PO}(p_y, -p_y) p_y^2 \left(1 - 2\frac{D}{L}\left(1 - \frac{D}{L}\right)(1 - \cos(q_y H))\right)$$

$$S_k^{OffSpec}(\vec{p}, \vec{k}) = A_s R_{PO}(k_y, p_y) p_y^2 \delta(Q_z) 2(1 - \cos(q_y H)) \times \\ \times \sum_{n=-\infty, n \neq 0}^{\infty} \delta(Q_x - 2n\pi) \frac{\sin^2\left(n\pi \frac{D}{L}\right)}{(n\pi)^2}$$

Phase-Object *Block Gaussian Distributed*

(Height H , Period L , Width D)

$$E\left(e^{iqH(\bar{r}_s)}\right) = e^{-\sigma^2 q^2 / 2 + i\mu q}$$

$$E\left(e^{iq_y(H(\bar{r}_{//} + \bar{r}_s) - H(\bar{r}_s))}\right) = e^{-q_y^2(\sigma^2 - C(\bar{r}_{//}))}$$

$$0 \leq x < D \quad C(\bar{r}_{//}) = H^2 \left(\frac{D-x}{L} - \left(\frac{D}{L} \right)^2 \right)$$

$$D \leq x < \frac{L}{2} \quad C(\bar{r}_{//}) = -H^2 \left(\frac{D}{L} \right)^2$$

$$C(0) = \sigma^2 = H^2 \frac{D}{L} \left(1 - \frac{D}{L} \right)$$

Sample surface correlation function:

$$G_s^{Spec}(\bar{p}, \bar{k}, \bar{r}_{//}) = G_s^{(0,0)}(\bar{k}) e^{-\sigma^2 q_y^2}$$

$$0 \leq x < D \quad G_s^{OffSpec}(\bar{p}, \bar{k}, \bar{r}_{//}) = G_s^{(0,0)}(\bar{k}) \frac{R_{PO}(k_y, p_y)}{R_{PO}(-p_y, p_y)} e^{-\sigma^2 q_y^2} \left(e^{q_y^2 H^2 \left(\frac{D-x}{L} - \left(\frac{D}{L} \right)^2 \right)} - 1 \right)$$

$$D \leq x < \frac{L}{2} \quad G_s^{OffSpec}(\bar{p}, \bar{k}, \bar{r}_{//}) = G_s^{(0,0)}(\bar{k}) \frac{R_{PO}(k_y, p_y)}{R_{PO}(-p_y, p_y)} e^{-\sigma^2 q_y^2} \left(e^{-q_y^2 H^2 \left(\frac{D}{L} \right)^2} - 1 \right)$$

Sample surface scattering function:

$$S_k^{Spec}(\bar{p}, \bar{k}) = \delta^2(\bar{Q}_{//}) A_s R_{PO}(-p_y, p_y) p_y^2 e^{-\sigma^2 q_y^2}$$

$$S_k^{OffSpec}(\bar{p}, \bar{k}) = A_s R_{PO}(k_y, p_y) p_y^2 \delta(Q_z) \times \sum_{n=-\infty, n \neq 0}^{\infty} \frac{H^2 q_y^2 \delta\left(Q_x - \frac{2n\pi}{L}\right)}{\left(H^2 q_y^2\right)^2 + (2n\pi)^2} \left[1 - \left(H^2 q_y^2 \frac{\sin\left(2n\pi \frac{D}{L}\right)}{2n\pi} + \cos\left(2n\pi \frac{D}{L}\right) \right) e^{-\frac{D}{L} H^2 q_y^2} \right]$$

Born Approximation

Similar to Phase-Object Approximation except that $R_{PO}(k_y, p_y)$ is replaced by

$$R_{FB}(k_y, p_y) = \frac{\Gamma^2}{4p_y^2(p_y - k_y)^2}.$$

2-D sample surface correlation function

According to Sinha³, for a reflectometer geometry (no angular resolution in the direction perpendicular to the beam and parallel to the sample surface, here the z -direction) the scattered intensity is given by the integral over Q_z (this was implicitly assumed in the previous, but there the sample surface correlation function was either in the z or x direction.). The resulting intensity is then given by the Fourier integral over the Q_x of the sample surface correlation function for $z = 0$.

DWBA *General*

Sample surface scattering function (which only holds if $S_k^{OffSpec}(\vec{p}, \vec{k})$ is integrated over Q_z):

$$S_k(\vec{p}, \vec{k}) = \int e^{-i\vec{Q}_\parallel \vec{r}_\parallel} G_s(\vec{p}, \vec{k}, \vec{r}_\parallel) d^2 r_\parallel$$

so

$$S_k^{Spec}(\vec{p}, \vec{k}) = 4\pi^2 A_s \left(\frac{\Gamma T(p_y)}{8\pi p_y} \right)^2 \delta^2(\vec{Q}_\parallel) \left| 1 + \frac{p_y}{p'_y} E \left(e^{-2ip'_y H(\vec{r}_s)} - 1 \right) \right|^2$$

$$S_k^{OffSpec}(\vec{p}, \vec{k}) = A_s \Gamma^2 \frac{T(p_y) T(k_y)}{8\pi |\kappa_y|^2} \delta(Q_z) \left\{ \int e^{-iQ_x x} E \left(e^{i(\kappa_y)^* H(x\vec{e}_x + \vec{l}_{se} + \vec{r}_s) - i\kappa_y H(\vec{r}_s)} \right) dx - 2\pi \delta(Q_x) \left| E \left(e^{-i\kappa_y H(\vec{r}_s)} \right) \right|^2 \right\}$$

According to eq. (7.14) of reference in footnote 2 the 2-shim count rate is proportional to this Sample surface scattering function integrated over the source area, detector area and sample area. The 2-flip count rate can be found in a similar way using eq. (7.16), where P_E in the ideal case (eq. (7.8) $P_R = 0$) is $\cos(Q_y l_{se})$, hence:

$$S_{k,flip}^{OffSpec}(\vec{p}, \vec{k}) = A_s \Gamma^2 \frac{T(p_y) T(k_y)}{8\pi |\kappa_y|^2} \delta(Q_z) \left\{ \int e^{-iQ_x x} E \left(e^{i(\kappa_y)^* H(x\vec{e}_x + \vec{l}_{se} + \vec{r}_s) - i\kappa_y H(\vec{r}_s)} \right) dx - 2\pi \delta(Q_x) \left| E \left(e^{-i\kappa_y H(\vec{r}_s)} \right) \right|^2 \right\}$$

while the specular part remains unchanged.

Similar expression can be derived for the Phase-Object and Born Approximations.

³ Sinha et al., Phys. Rev. B **38** (4) 1988, p2297-2312

Appendix D: Self-Affine Gaussian correlation function and its

Fourier transform.

The Self-Affine Gaussian correlation function is defined as:

$$C_{SA}(\vec{r}_{//}) = \sigma^2 e^{-(r_{//}/\xi)^{2h}},$$

where σ = standard deviation of distribution, h is the jaggedness parameter and ξ is the correlation or cut-off length. The expectation value of such a distribution is given by:

$$E\left(e^{iQ(H_{SA}(\vec{r}_{//} + \vec{r}_s) - H_{SA}(\vec{r}_s))}\right) = e^{-Q^2(\sigma^2 - C_{SA}(\vec{r}_{//}))},$$

The specular part of the scattering can be calculated from the standard deviation alone, according to the formulas in Appendix C. The off-specular part is proportional to the Fourier transform of :

$$e^{-Q^2 C_{SA}(\vec{r}_{//})} - 1,$$

where $Q = |\kappa_y|$ for DWBA and $Q = q_y$ for Born approximation and Phase-object approximation. According to R. Pynn (Phys. Rev. B, Vol.45, No 2, January 1992 p602-612) As long as $q_y^2 \sigma^2 < 1$, a reasonable approximation of this value is found by inserting

$$e^{-Q^2 C_{SA}(x)} - 1 = \alpha^2 e^{c_0(\alpha, h) - c_1(\alpha, h) \frac{x}{\xi} - c_2(\alpha, h) \left(\frac{x}{\xi}\right)^2},$$

where $\alpha = Q\sigma$, $c_1(\alpha, h)$ and $c_2(\alpha, h)$ are parameters which depend only weakly on α but strong on h , and $c_0(\alpha, h)$ depends weakly on h and stronger on α . Pynn does not give values for these coefficients but it can be found that a reasonable approximation is given by:

$$c_0(\alpha, h) = \frac{\alpha^2}{4} + \frac{\alpha^4}{16},$$

$$c_1(\alpha, h, \xi) = \frac{1}{\xi} \left[\frac{\alpha^2}{\pi} + \frac{1-h^2}{\beta(h)} \right],$$

$$c_2(\alpha, h, \xi) = \frac{1}{\xi^2} \left[1 - \frac{1-h^2}{\beta(h)} \right] + \frac{1}{2\sigma_{coh}^2},$$

$$\beta(h) = \max\left[\frac{2}{e}, 1-h^2\right],$$

where σ_{coh} is the coherence length defined as the standard deviation of the Gaussian Resolution distribution of the neutron or X-ray beam:

$$I(x) = I_0 \frac{e^{-\frac{1}{2}\left(\frac{x}{\sigma_{coh}}\right)^2}}{\sigma_{coh} \sqrt{2\pi}} .$$

The Fourier transform of this approximate function is a Voight function, which can be calculated by means of the complex error function. However, it can also be approximated by a sum of a weighted Lorentzian and Gaussian distribution, with different width. The way this is done is shown by P. Thomson et al. (J. Appl. Cryst. **20** (1987) p79-83) and G. K. Wertheim et al. (Rev. Sci. Ins. **45** (11) (1974) p1369-1371).

$$\int_0^{\infty} \cos(q_x x) I(x) \left(e^{-Q^2 C_{sd}(x)} - 1 \right) dx =$$

$$= \frac{I_0 \alpha^2 e^{c_0(\alpha, h)} e^{-c_1(\alpha, h) \frac{x}{\xi} - c_2(\alpha, h) \left(\frac{x}{\xi}\right)^2}}{\sigma_{coh} \sqrt{2\pi} \Gamma} \left[\frac{\eta}{1 + 4 \left(\frac{q_x}{\Gamma}\right)^2} + (1 - \eta) \sqrt{\pi \ln(2)} e^{-4 \ln(2) \left(\frac{q_x}{\Gamma}\right)^2} \right],$$

where

$$\Gamma = \left(\Gamma_G^5 + 2.69269 \Gamma_L \Gamma_G^4 + 2.42843 \Gamma_L^2 \Gamma_G^3 + 4.47163 \Gamma_L^3 \Gamma_G^2 + 0.07842 \Gamma_L^4 \Gamma_G + \Gamma_L^5 \right)^{\frac{1}{5}},$$

$$\eta = 1.36603 \frac{\Gamma_L}{\Gamma} - 0.47719 \left(\frac{\Gamma_L}{\Gamma} \right)^2 + 0.11116 \left(\frac{\Gamma_L}{\Gamma} \right)^3,$$

$$\Gamma_G = 2 \sqrt{\ln(2)} \sqrt{c_2(\alpha, h, \xi)}, \quad \Gamma_L = c_1(\alpha, h, \xi).$$

The 2-flip count rate can be found in a similar way, where the approximation is used:

$$\int_0^{\infty} \cos(q_x x) I(x) \left(e^{-Q^2 C_{sd}(\sqrt{x^2 + l_{se}^2})} - 1 \right) dx =$$

$$\frac{I_0 \alpha^2 e^{c_0(\alpha, h) - c_1(\alpha, h) l_{se} - c_2(\alpha, h) l_{se}^2}}{\sigma_{coh} \sqrt{2\pi} \Gamma} \left[\frac{\eta}{1 + 4 \left(\frac{q_x}{\Gamma}\right)^2} + (1 - \eta) \sqrt{\pi \ln(2)} e^{-4 \ln(2) \left(\frac{q_x}{\Gamma}\right)^2} \right]$$

while the specular part remains unchanged.