

Scatter

Version 2.5

March 2011

User guide

Preamble

Scatter is a program intended to analyse Small-Angle X-ray Scattering (SAXS) and Small-Angle Neutron Scattering (SANS) data either by comparing the measured 2D pattern with a simulated one, calculated using a theoretical model of the structure under test, and/or by performing an adaptive fitting of the scattering curve obtained after reduction of the raw 2D data.

The program is a standalone executable that runs in Windows environments. So far, it has been successfully tested on PCs running Windows 2000 and Windows XP.

Getting started with *Scatter*

Double-clicking on *Scatter.exe* opens the main Graphical User Interface (GUI). From it, the user can load, display and analyze:

- 1D data (scattering curves) using a general GUI (button *1D scattering curve*). As stated in the preamble, in this case it is assumed that data reduction has already been done
- 2D data (scattering patterns), using the general GUI opened by the *2D scattering pattern* button.

The program assumes number to be entered in the format 11234.334, i.e. the decimal delimiter is a point, and not a comma. In some cases, this has to be adjusted in the Windows country options.

1D data analysis, simulation, and fitting

In this GUI of *Scatter* the user can load the 1D reduced data in order to display and compare them with a simulated curve according to a chosen model. After choosing a reasonable model for the data, the user can initialize the model parameters and start the fitting operation.

Data formats

Scatter is able to read 1D ASCII data written column-wise according to the following conventions:

- **.txt* or **.out*: raw reduced SAXS data or Gradzielski-like format, specific to beam-line ID02 at the ESRF. Such a file contains two or three columns of values corresponding to q and $I(q)$, or to q , $I(q)$ and $err(q)$ respectively, separated by a *Tab* character or by one or more whitespaces. In the Gradzielski format, data is preceded

by a header of about fifty lines, each of them starting with a # character. If $err(q)$ is not provided explicitly, its value is estimated in Scatter as $I(q)/100$.

- *.csv: comma-separated values of q , $I(q)$, and $err(q)$. Similarly, $err(q)$ is estimated as $I(q)/100$ if not provided explicitly. Blanks are tolerated between a comma and the next value on a line. The file has no header.
- *.pri, *.mul, *.sub, *.fun: blank-separated q , $I(q)$, and $err(q)$ values, preceded by a 5-lines header.
- *.asc: Tab-separated q and $I(q)$ values. The first line is skipped since it just says who's who. $err(q)$ has to be estimated like for the other formats.
- *.uxd: blank-separated q and $I(q)$ values, after a 57-lines header. Again, $err(q)$ is estimated afterwards by the program.
- *.chi: fit2d output. The format is similar to *.uxd, excepting that the header has only 4 lines.
- *.csw is a comma-separated data format specific to Scatter. It is used to save the evolution of a set of ten parameters while analyzing the data: x_axis , I , dI , qu , qv , $angle$, qx , qy , qz , and the cut type (horizontal, vertical or circular).

Loading and plotting the 1D data

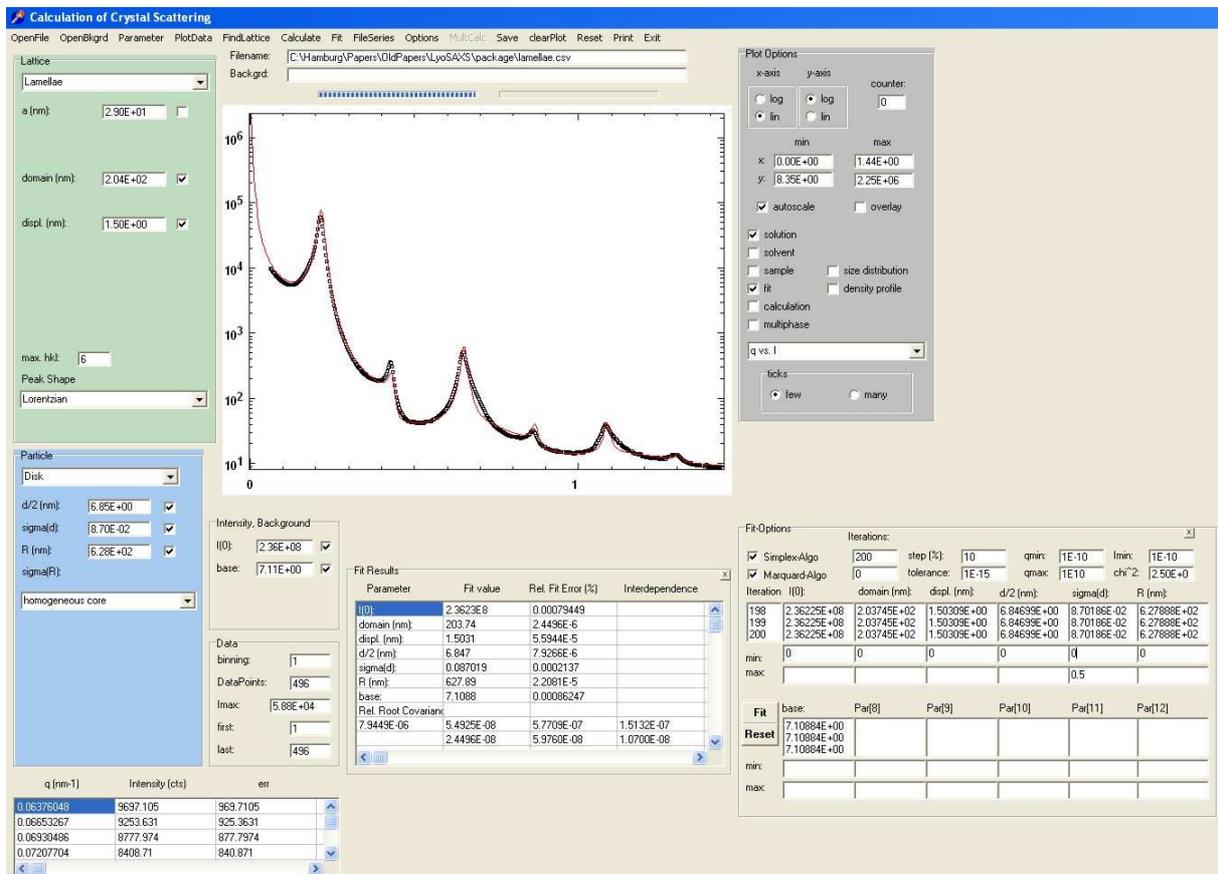


Fig. 1: GUI for the 1D-data treatment

Simulation and adjustment of parameters

Once your data are loaded and displayed as required, you can simulate curves according to several theoretical models. In order to display in the main plot the scattering profile of the theoretical model, you have to choose the particle shape (sphere, cylinder, etc...), the particle nature (homogeneous, core-shell, etc....) and the kind of lattice (FCC, BCC, none, etc...). You can do this by checking the correct options in the *Crystal Lattice*, *Particle* and *Particle interior* boxes. Once the model has been chosen, you can simulate the corresponding scattering profile by pressing the *Calculate* button. To adjust the profile height with respect to your experimental data, use the $I(0)$ parameter. In case of a constant background, the *baseline* value can be adjusted as desired.

Numerous models are available and the basic information, including some fundamental references, are listed below.

Particle Structures

Formfactors for different particulate structures such as spheres, cylinders, lamellae (disks), vesicles, liposomes, Kratky-Porod-chains and excluded volume chains can be calculated. Anisometric particles (cylinders, disks) are assumed to have an isotropic orientational distribution. The particles are schematically shown in Fig. 1.

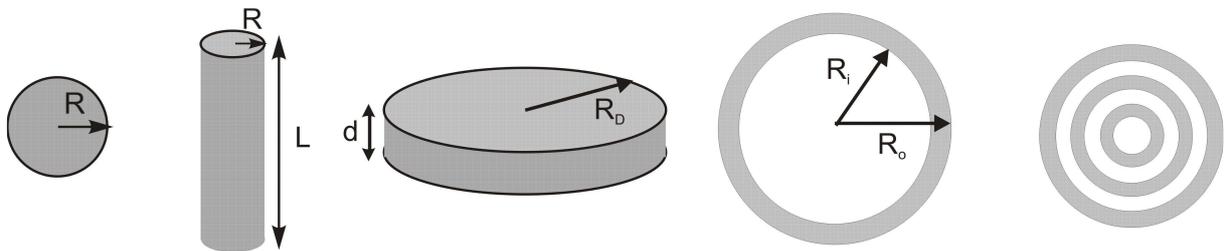


Fig. 2: Particle shapes that are used in Scatter.

Particles can have a core/shell-structure consisting of a homogeneous core, and a homogeneous or inhomogeneous shell.

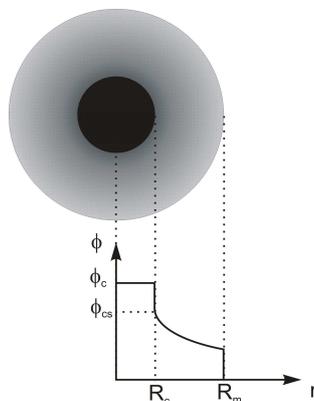


Fig. 3: Cross-sectional density of core/shell-particles

Inhomogeneous shells are assumed to have a density profile of the form $\phi \sim r^{-\alpha}$, i.e. a scaling law typical for polymer brushes. The value of α depends on the geometry (spherical, cylindrical, or planar polymer brush) and the solvent quality. A value of $\alpha = 0$ corresponds to a homogeneous shell. Further, the ratio $\rho = \phi_{cs}/\phi_c$ of the shell and the core density at the interface have to be specified.

Spheres

You need to specify

- the sphere radius R and
- its relative standard deviation σ .

For homogeneous core/shell particles in addition

- the outer radius R_m and
- the density ratio ρ have to be given.

For inhomogeneous shells further

- the parameter α has to be specified.

For spherical polymer brushes this parameter has typical values between 1 (theta solvent) and 4/3 (good solvent).

Cylinders

You need to specify

- the cross-sectional radius of the cylinder R ,
- its relative standard deviation σ , and
- the length of the cylinder L .

The scattering curve is calculated for isotropic distribution of cylinders. For homogeneous core/shell cylinders in addition

- the outer radius R_m and
- the density ratio ρ have to be given.
- For inhomogeneous shells further the parameter α has to be specified.

For cylindrical polymer brushes this parameter has typical values of 2/3.

Lamellae

A lamella is modelled as a disk of thickness $d=2R$ and a lateral radius R_D . You need to specify

- R (i.e. half its thickness),
- its relative standard deviation σ , and
- the lateral radius R_D .

The scattering curve is calculated for an isotropic distribution of disks. For homogeneous core/shell particles in addition

- the outer radius R_m and
- the density ratio ρ have to be given.

For inhomogeneous shells further

- the parameter α has to be specified.

However, for planar polymer brushes this value is typically equal to zero corresponding to a homogeneous shell. In this case, the calculation should be performed for the homogeneous core/shell-case which is much faster.

Vesicles

You need to specify

- the radius R_i to the inner rim of the bilayer, and
- the radius R_o to the outer rim of the bilayer.

The bilayer thickness is then equal to $D = R_o - R_i$. Further you need to specify

- the relative standard deviation of the vesicle radius σ_R and
- the relative standard deviation of the bilayer thickness σ_D .

Liposomes

A liposome is understood as a multi-lamellar vesicle with an onion-like structure. As for the vesicle you need to specify

- the radius R_i to the inner rim of the bilayer,
- the radius R_o to the outer rim of the bilayer,
- the relative standard deviation of the vesicle radius σ_R , and
- the relative standard deviation of the bilayer thickness σ_D .

In addition you need to specify

- the number of concentric vesicles (shells), i.e. the lamellarity.

All shells are assumed to have the same distance with respect to each other.

Kratky-Porod Chains

For the Kratky-Porod chain you need to specify

- the contour length L and
- the persistence length l_p .

For an infinitely thin Kratky-Porod chain you select *none* for the internal structure. If the Kratky-Porod chain has a finite thickness, then

- the radius R and
- its relative standard deviation σ have to be specified.

For inhomogeneous chains further

- the outer radius R_m and
- the density ratio ρ have to be given.

For inhomogeneous shells further

- the parameter α has to be specified.

For cylindrical polymer brushes this parameter has typical values of 2/3.

Excluded Volume Chains

For the excluded volume chain you need to specify

- the radius of gyration R_g ,
- the Flory-exponent ν and
- the parameter γ .

Cube

You need to specify

- the cube edge length
- its relative standard deviation σ .

2D-data/orientational distribution functions

When 2D-data sets are considered, i.e. horizontal, vertical, or azimuthal slices through 2D-data generated with crystal3d, in addition

- the relative standard deviation of the cylinders or disks σ_L have to be specified.

Further, the orientational distribution of the cylinders has to be given. For this several orientational distribution functions can be chosen such as an isotropic distribution, all cylinders or disks oriented in the z -direction, and further Gaussian, exponential, Onsager, Maier-Saupe, Heaviside, or Laguerre-type distribution functions.

For the orientational distribution functions

- the average angle $\bar{\delta}$ (*dbeta*) has to be specified.

The orientational distribution functions for typical values are shown in Fig. 22.

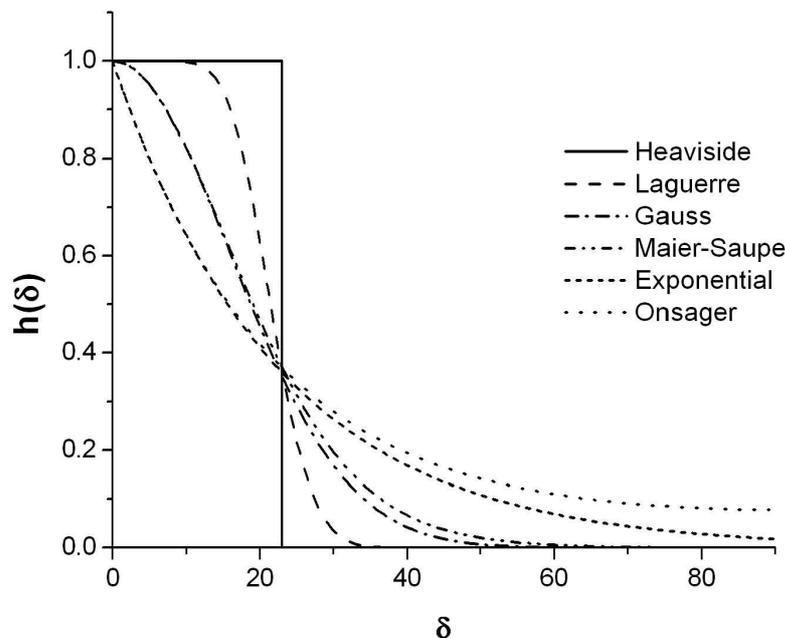


Fig. 4: Orientational distribution functions used in Scatter.

Lattices

A number of different lattices can be calculated such as lamellae, cylinders packed in hexagonal, square or centered rectangular lattices, bcc, fcc, sc, hcp and body-centered tetragonal structures (bct), ordered bicontinuous structures such as the gyroid (Ia3d), double diamond (Pn3m), plumbers nightmare (Im3m), random close-packed-layers, Percus-Yevick liquid-like structures, fractal-like aggregates and two-dimensional arrangements of spheres or cylinders typical for GISXAS/GISANS-experiments.

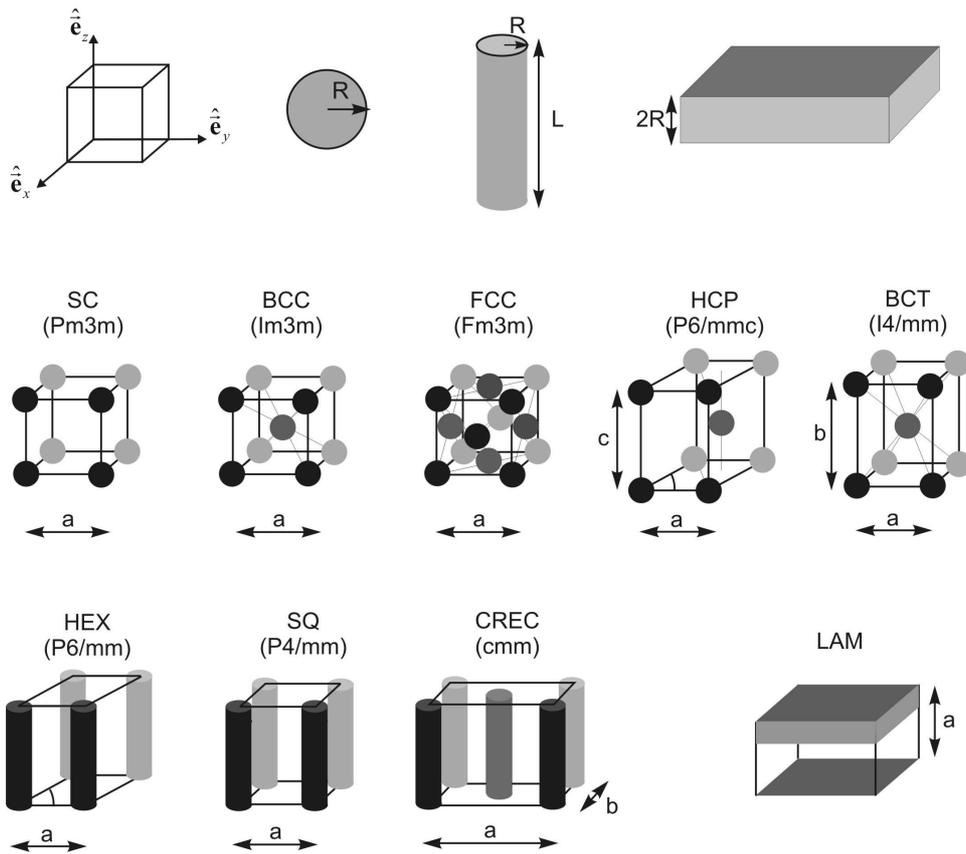


Fig. 5: Lattice types available for calculations

For each of the structures

- the unit cell dimension a (and possibly b),
- the average domain size,
- and the average displacement from the ideal lattice point (Debye-Waller factor)

need to be specified. The average domain size is inversely proportional to the peak width. Large displacement values will diminish the intensities of the higher order reflections. Further

- a maximum hkl -value should be given.

The number can be arbitrarily large, but this will slow down the calculation.

Further a peak shape can be selected, for which different peak shape functions are available such as Gaussian and Lorentzian peaks, modified Lorentzians 1 and 2, the Pseudo-Voigt, the Pearson-VII and a generalized Gamma-function. The last three function require to

- specify an additional parameter that can have values between zero and one for the Pseudo-Voigt and the Pearson-VII function, and values between 0 (=Gaussian) and infinity (Lorentzian) for the generalized Gamma function.

The anisotropic Gaussian function is only applicable to 2D-data sets.

The calculations for the bicontinuous structures are done in an approximation, where vesicles are arranged on body-centered ($Ia3d$, $Im3m$) or simple cubic ($Pn3m$) lattices such that the hydrophilic/hydrophobic volume fractions correspond to the correct values. As a consequence the relative intensities of the higher order reflections are not correct, but the positions are.

Data analysis

Plotting your data

A typical data analysis would proceed as follows. The data file is loaded with *OpenFile*. The program will autoscale the data and display them in an image. The minimum and maximum values of x (q -axis) and y (intensity-axis) are given in the grey *Plot Option* box on the right of the image. The number of data points and the maximum intensity are given in the *Data box* below the image.

You can choose different ways how to plot your data in the *Plot Option* box. Clicking on *x-axis log* will automatically plot the data on a logarithmic x -axis. Similarly you can choose *x-axis lin*, *y-axis lin*, or *y-axis log*. In the *Plot Option* box instead of *q vs I* you can further select other types of plots such as Guinier, Zimm, Holtzer, Kratky or Porod plots just by clicking onto them. For the Guinier plot the program will automatically do a linear regression to give you the radius of gyration, its relative error, the radius of an equivalent sphere, and the correlation coefficient of the fit in the *Fit Results* box below the image. By adjusting the first and last data point to be considered for the regression in the *Data* box, and clicking on *PlotData* (or *Ctrl D*), the regression only considers the values indicated in black, and ignores the data indicated in blue. The results of the new regression are again given in the *Fit Results* box.

Similar the Zimm-plot will automatically make a linear regression to give you the intercept, from which the molecular weight could be calculated, and the slope, from which the radius of gyration could be calculated. However, for these calculations the intensity on absolute scales as well as the optical constants of the experiment have to be known. The Holtzer-, Kratky-, and Porod-plots will automatically fit a horizontal line through the data, from which the mass per unit length (Holtzer) or the internal surface area (Porod plot) could be calculated, given that the intensity is on absolute scales and that the optical constants are known.

To choose a particular range for plotting your data, you can deselect autoscale and enter the desired values in the x (min/max) and y (min/max) fields, and click *PlotData* (or *Ctrl D*).

Often, measured background, e.g. scattering of the solvent, has to be subtracted from the data. The background file is loaded by selecting *OpenBkgrd*. The program assumes that the background file has the q -values as the data file. The program then displays the background data in green together with the data in the image. Further it subtracts the background from the data and displays the *Sample* data in red also in the image. The factor by which the background is multiplied and subtracted from the data is by default equal to one, but can be changed in the *Intensity/Background* box below the image. This factor can also be fitted if the *subtract* checkbox is checked. If background is loaded, all regressions in the Guinier, Zimm, Holtzer, Kratky and Porod-display apply to the *sample* data (in red).

The plot can be cleaned by pressing the *clearPlot* button.

Modelling your data

You can start modelling your data by choosing a *Lattice* and a *Particle* and enter the required parameters. You further have to specify the intensity (proportional to the primary beam intensity) and a horizontal flat background in the *Intensity, Background* box just below the

image. By clicking on *Calculate* (or *Ctrl C*) the program will calculate the corresponding scattering curve and display it together with the data. The progress of the calculation is displayed in the progress bar above the image. Calculations can be very fast in case of spheres, but also slow in case of cylinders, or inhomogeneous core/shell structures, where the calculations are mathematically more demanding. You can interrupt any calculation by pressing the *ESC*-button. By choosing some lattice/particle model and adjusting the parameters one can quite often get some first reasonable agreement between the calculation and the experimental data.

If calculations have been performed, the program allows one to plot the size distribution of the particles by checking the *size distribution* box in the *Plot Options* box and selecting *PlotData* (or *Ctrl D*). Similarly by checking the *density profile* box and selecting *PlotData* (or *Ctrl D*), the density profile is displayed. One should choose only one of both check boxes. If both are checked, then only the size distribution is displayed.

Fitting your data

If there is reasonably good overlap between the data and the calculation, one can start fitting the model calculation to the data set. For this one can select the first and the last data point to be considered in the *Data* box. After clicking on *PlotData* (or *Ctrl D*) the data points to be considered are displayed in black, the other data points in blue. Then select *Fit* → *Initialize* in the main menu. It displays the *Fit Option* group box where the number of iterations for the Simplex-fit and the number of iterations in the subsequent Levenberg-Marquardt-fit can be specified. Further you can specify minimum and maximum *q*-values (*qmin*, *qmax*) to be considered, and the minimum intensity (*Imin*). In the *Fit-Options* box you can limit the range of a number of parameters to physically or mathematically plausible ranges. For the first fit default values are used.

To obtain a first good fit to your data, one can do the following. Choose a small number of iterations, e.g. 20, for the simplex fit and zero iterations for the Marquardt fit. If Marquardt fit is checked with zero iterations, the Marquardt algorithm will just give you an estimate of the fit error, but will not fit further. The range limitations of the parameter are only taken into account in the simplex fit. By checking the boxes next to the parameters in the Lattice, Particle and Intensity box, you select the parameters to be fitted. At the beginning, choose only a few, i.e. 1-3 parameters such as intensity, particle radius, peak width to see if the fit converges. By clicking *Fit* → *Fit*, *Ctrl F*, or the *Fit*-button you start the fitting procedure. The left progress bar shows you the progress in the fit. If you decide to interrupt the fit, just press the *ESC*-button. In the *Fit-Option* group box the number of the current iteration, the current fit values of the fitted parameters are displayed. The simplex algorithm stops automatically, if the relative tolerance gets below a preset value of 1E-15. After completion of the fit, the program will plot the fitted function and lists the fitted values in the *Fit Results* box together the relative fit error obtained from the covariance matrix generated by the Marquardt-algorithm. Also, the covariance matrix (upper right half) is displayed. If parameters are not statistically independent from each other, a '#' is displayed in the corresponding lines. In this case you should lower the number of fitted parameters to have better statistical significance of the fitted values. The old parameters are overwritten by the new fitted values. If the fit results are unacceptable, you can get back the old parameters by clicking *Reset* in the main menu or the *RESET* button in the *Fit-Option* group box. If the fit was successful, you can fit more and finally all parameters of your model and choose a sufficient number of iterations. You can save the calculation or the fit by clicking *Save* → *SaveCalculation* and *Save* → *SaveFit*. The files are stored in Excel-format (comma-separated) and you have to add *.csv as the extension.

If you just want to display your data together with the fit, you deselect *calculation* in the *Plot Options* box. You can store the plotted image as a bitmap by selecting *SaveImage*. Here you need to add the extension *.bmp.

If the fit takes very long, you can bin the data by choosing an appropriate number of data to bin in the *Data* box, before loading the data. Choosing 4 means that 4 subsequent (q, I)-values are averaged to get one data point. A smaller number of data points will considerably speed up the fitting procedure.

Many times it is just not possible to obtain an acceptable fit. There can be many reasons such as that the assumed model is incorrect, numerical problems during the calculations, parameters with unphysical values etc. Often one can still manually adjust the parameters to obtain a reasonable agreement with the data and store the calculated curve with *SaveCalculation*.

Series fitting

The program allows to automatically fit large number of data files such as files from time-resolved studies. A requirement is that subsequent scattering curves do not differ too much, so that the fitted values of the first curve can be used as starting parameters for a fit to the next curve. Before starting a fit series, choose the first data file and perform a fit so that the parameter values are set to an optimal start value. The first/last point, *qmin/max* and *Imin* for the fit will apply to all data sets.

The program assumes that your file series has a consecutive numbering in the file name, e.g. *samplename001.ext*, *samplename002.ext*, ... *samplename423.ext*. To tell the program where in the filename the consecutive numbers are contained, you select *FileSeries* and click *Choose File format*. In the new box below the image check the positions in the file name, where the numbering occurs. You can choose up to 4 positions, so that a maximum of 10000 files can be fitted. To first check if the files can be properly loaded, first select *FileSeries* and click *ViewFileSeries*. Then the program asks you to select the first file and the last file of this series. It then displays these files in the image. The name of the first file is displayed in the *FileName* box above the image, the name of the last selected file in the *Backgrd* box above the image.

By selecting *FileSeries* and clicking on *FitFileSeries* you select the first and the last file to be fitted. Then the program is automatically loading each file, fitting the data, plotting the fit, and writing the fitted values in a matrix. After the fit, the program asks you for a filename, where the fitted parameters should be stored. The file is written in Excel-format (*.csv). It contains the consecutive number, the fitted parameters, the relative fit errors and a warning, if the parameters are not independent. This file cannot e.g. be directly imported into Excel or Origin to display selected parameters for the whole series of data sets.

If there is no consecutive numbering in the file names, you can store the files in a separate folder. With *ViewFolder* and *FitFolder* you can perform the same series fitting as above.

Storing and loading parameter files

All parameter values and settings can be stored in a parameter file that can be loaded later to proceed with the analysis. For saving the parameters select *Parameter* and click on *SavePar*

to choose a filename. The extension should be *.par. This parameter file can be loaded by selecting *Parameter* and clicking on *OpenPar*.

Multiphase calculations

By selecting *Options* and clicking on *Multiphase Systems* a new box right to the *Plot Options* box appears. You can add three different scattering curves to a resulting scattering curve. By selecting *Phase 1*, all subsequent calculations will be stored as Phase 1. By selecting *Phase 2*, all subsequent calculations will be stored as Phase 2, and similarly for *Phase 3*. The three phases are added in proportion to the coefficients given in the *Intensity* fields. For the calculation click *MultCalc*. The calculation can be stored by selecting *Save* and clicking on *MultiPhase*.

2D data analysis and simulation

Data formats

Scatter can handle several specific image formats:

- EDF (ESRF/Klora data format), BSL/OTOKO,
- raw and T-files output by ILL scattering beam-lines,
- AIDA (*.pcb) used by some image plate detectors,
- spreadsheet (ASCII) 2D data generated by program *Fit2D* (*.spr),
- *.img format as used at the ALS (Berkeley Lab),
- Pilatus *.cbf and *.tif formats
- common formats like Bitmap (*.bmp), 8-bit and 16-bit TIFF, and PNG.

Anisotropic structures (crystal3d)

Spheres

You need to make the same specifications as in the isotropic case.

Cylinders

For the anisotropic case you need in addition to specify the relative standard deviation of the cylinder length and the orientational distribution of the cylinders. There is a choice of orientational distribution functions. They are discussed below. The cylinders are ideally assumed to be oriented in the z-direction (001).

Lamellae

For the anisotropic case you need in addition to specify the relative standard deviation of the lateral disk radius and the orientational distribution of the disks. There is a choice of orientational distribution functions. They are discussed below. The disks are ideally assumed to be oriented with their normal in the z-direction (001).

Vesicles

You need to make the same specifications as in the isotropic case.

Liposomes

You need to make the same specifications as in the isotropic case.

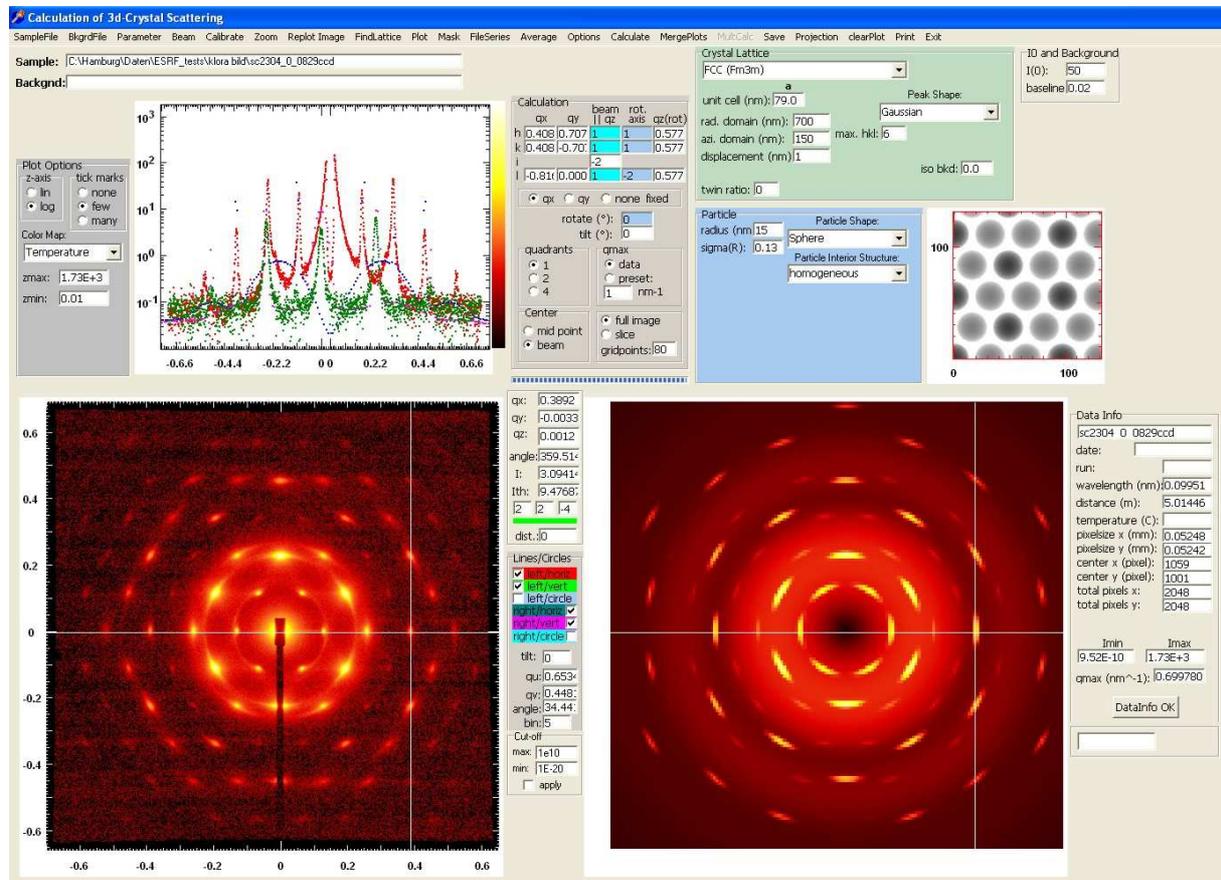


Fig. 6: GUI for the analysis of 2D-data

Analyzing scattering patterns

Scatter is currently the only software that allows one to simulate the SAXS pattern of a given sample using a theoretical model, and to compare the result with the experimental 2D data. In the following, we will present the steps of the analysis using as an example a pattern obtained at the ESRF on beam-line ID02.

After clicking on *2D (scattering pattern)* you enter the graphical user interface (GUI) for the analysis and modeling of 2-dimensional data. Double-clicking on the blue upper frame will display the graphical user interface in full size.

Loading your data

In a typical analysis you first select *SampleFile* in the main menu and select a file type. These are typical detector files from beamlines at ESRF, ILL, and HASYLAB/DESY. If your file type is not among the list, you may use *Fit2D* to open your file and export it in a spreadsheet format (*.spr). This file type is among the selections in the list.

Every specific data format has its own entry that calls a dedicated procedure. Note that for BSL data you must select the header file (*Xnn000.mdd*) as input; it contains all the information needed to load the 2D data. Sub-menu *Other formats* can handle *.png, *.bmp, and 16-bit TIFF images. After selecting the file type, you can open your data file using a standard Windows *Open* dialog box. A progress bar placed below the *Calculation* box illustrates the evolution of data loading.

Data display

After selecting your file, it will be displayed in the lower left image (*Data Image*) in a 512 x 512 pixel window. If the original image is larger or smaller than these dimensions, it will be stretched or reduced so as to fit the given area. The aspect ratio is maintained.

The intensity is by default on a logarithmic scale and autoscaled. You can change the plotting options in the upper left group box *Plot Options*. You can adjust the minimum and maximum values of the intensity, a linear or logarithmic presentation and choose a color map. Changes in the log/lin-option and the color map lead automatically to replotting of the whole image. After adjustment of the min/max-values you can replot the image by selecting *Replot Image* in the main menu. You can also choose whether tick marks and tick labels should be displayed. The upper image (*Analysis Image*) displays the intensity scale on the left together with the corresponding color scale on the right for quantitative comparison.

To update the *Data Image*, click *Replot Image*. Note that when the image is redrawn after having modified *zmin* and/or *zmax*, the new intensity range is mapped onto the entire color-map range.

The q-scales are calculated from the data parameters in the *Data Info* group box. Parameters that are relevant for the calculation of the q-scales are the wavelength, the sample-detector distance, the pixel size, the beam position, and the number of pixels on the detector. These data are sometimes provided by the data file (e.g. in case of *.edf) and are read from the data header. If not, default values are used to display a default q-scale. In this case the default parameter values and the q-values are colored in red. The user is expected to enter the correct values in the *Data Info* group box. The beam position, sample-detector distance and wavelength can be determined using the beam centering and calibration routines. If the correct values are entered, this is confirmed by pressing the *DataInfo OK* Button. Then all parameters and q-values are displayed in white.

In addition to those parameters already mentioned, one can find in the *Data Info* group box a description of the sample, the date of the experiment and the run number (if any), the sample temperature during acquisition, the range of the average intensity in the image, and the q_{max} .

Background Subtraction

Often background has to be subtracted from the measured data. For loading the background data select *BkgrdFile* from the main menu, select the file type and then the file. The background data are then displayed in the lower right image. For plotting the background data the same plot settings in the *Plot Options* group box are used that were specified for the data file. The background file can be subtracted from the data file by checking the *sub* checkbox in *Plot Options* and specifying the *prefactor* for the background data. It is by default set to 1.0. If due to differences in primary beam intensity or measurement time this prefactor is different

from unity, it can be adjusted accordingly. By selecting *Replot Image* from the main menu, the subtracted data file is shown in the *Data Image*. As long as the *sub* checkbox is checked, all calculations will be performed on the background subtracted data.

Beam position

Usually, the beam position (in pixels) is already known and can be entered in the *DataInfo* group box. The most direct way is to collect an image of the attenuated beam on the detector and determine its center. If not possible, one has to deduce the beam position from scattering patterns. For both procedures existing data reduction and analysis software packages (e.g. Fit2D) provide appropriate tools. If the beam position is not known, then Scatter provides some means for the determination of the beam position.

To determine the beam position on the detector, select *Beam* from the main menu. For the specification of the beam position the *Data Image* is enlarged for higher accuracy. There are four options to determine the beam position. By choosing *Beam* → *Manual* you can click with the cursor on the beam position. The selected beam position (in pixels) is displayed in the *Data Info* group box and it is indicated by a white cross in the *Data Image*. If the cursor is moved away from the beam position, also a white circle around the beam position is displayed. The intensity along this circle is displayed in the *Analysis Image*. By comparing the position of peaks or Debye-Scherrer rings with the circle it is possible to check whether the selected beam position is correct. If not, a better position can be selected by clicking on the *Data Image*. If the position is acceptable, click *Beam* → *Accept beam position* in the main menu. Then the image is replotted with the new beam position.

Another option is to use trackbars by selecting *Beam* → *Center with trackbar*. This option can be used when the scattering pattern is *isotropic* or when the upper/lower half and left/right half are *symmetric*. By selecting track bars, one track bar on top of the *Data Image*, and one on the left side of the *Data Image* are displayed. By dragging the rider to the left or right on the upper trackbar, the intensity along horizontal cuts through the *Data Image* at the vertical position of the left trackbar are displayed in the upper image. The intensity towards the right side of the beam center, indicated by the white cross, is displayed in red, the intensity towards the left side of the beam center is displayed in green. When the two cuts superimpose, the beam center is in the appropriate position. The pixel position is given in the *DataInfo* group box. The same procedure is then used for the track bar on the left side of the *Data Image*. Dragging it up and down will shift the beam position accordingly. The intensity towards the upper side of the white cross is displayed in red, the intensity towards the lower side is displayed in green.

A third option is to use data points on a circle around the beam position by selecting *Beam* → *Center with circle*. This option can be used for samples with circular Debye-Scherrer rings (e.g. silver behenate calibration sample) or samples with a set of Bragg peaks that are located on a circle. This is the most accurate way to determine the beam center. After selecting the *Beam* → *Center with circle* option, one has to click at least on three points (maximum six points) on a circle. After clicking on the third point, the beam position will be displayed by a white cross. The position of the center (in pixels) is displayed in the *DataInfo* group box. One can select six points in total. One can follow, if the position of the beam as indicated by the white cross and the pixel values in the *DataInfo* box are changing any more if more points are selected. If the beam position is unacceptable, the RESET button displayed on the lower left of the *Data Image* can be clicked.

A fourth option is to calculate the center of gravity of the *Data Image* by selecting *Beam* → *Center of gravity*. This option can only be used if the data image is symmetric with respect to the beam position. Usually, already the shadow of the beam stop holder will lead to non-symmetric images. After selection, the beam position is indicated in the *DataInfo* group box.

If the selected beam position is acceptable, select *Beam* → *Accept beam position*. This avoids that further clicking in the *Data Image* will alter the selected beam position.

For GISAS patterns often the primary beam does not hit the detector and therefore its position cannot be determined from the measured 2D-data. In this case the primary beam position is calculated from the position of the reflected beam. After selecting 2DHex (GISAXS) from the Lattice group box, a field for the incident angle appears in the *DataInfo* group box. After selecting *Beam* → *Manual* or *Beam* → *Center with Trackbar* the position of the reflected beam can be specified. A white cross corresponding to the position of the reflected beam and a white cross corresponding to the calculated position of the primary beam are shown. The position of the primary beam is then displayed in the *DataInfo* group box.

Calibration

Usually, the experimental parameters from which the scattering vector is calculated, i.e. pixel size, sample detector position, wavelength, are known and can be entered in the *DataInfo* group box. Assuming that at least the pixel sizes are known, *Scatter* provides some tools to determine the wavelength (then sample-detector distance has to be known) or the sample-detector distance (then wavelength has to be known) from measured calibration samples such as silver behenate or rat tendon. This is also a means to check for consistency, if all parameters are known.

For calibration the measured scattering pattern of the calibration sample is loaded into the *Data Image*. For calibrating scattering patterns it is good to display the intensity on a log-scale and adjust the min/max-values such as to clearly see as many reflections as possible.

To calibrate the wavelength select *Calibrate* → *Calibrate Wavelength* and then select the calibration sample. The wavelength is then calculated by assuming a given pixel size and sample-detector distance whose values have to be given in the *DataInfo* group box. The calibration proceeds by clicking on the reflections in the *Data Image*. Before clicking on the first reflection, the order of the first reflection has to be given in the *Calibration* group box at the lower right side of the *Data Image*.

Since the position of the lowest order reflections can be affected by the strongly increasing diffuse scattering around the beam stop, the best results are usually obtained by selecting high intensity higher order peaks, e.g. 6th and 9th order of rat tendon patterns. After the first click the calculated wavelength is given in the *DataInfo* group box. For further peak selections the order of the reflections is calculated and given in the *Calibration* group box. It should be checked for correctness. An arbitrary number of reflections can then be clicked on and checked in the *DataInfo* group box, if the calculated wavelength stays consistently in a small range of values.

For calibrating the sample-detector distance select *Calibrate* → *Calibrate detector distance* and choose the appropriate calibration sample. Also in this case the order of the first reflection

has to be given. For further selected reflections the order is calculated and the derived sample-detector distance given in the *DataInfo* group box.

If the calibration is acceptable, select *Calibrate* → *Accept calibration* in the main menu.

After determination of the beam position and calibration, all parameters in the *DataInfo* group box can be accepted by clicking on the *DataInfo* o.k. button in the *DataInfo* group box. Then all parameter and q-values that had previously been displayed in red are displayed in white. Further the *Data Image* is replotted with the valid q-scale on the qx- and qy-axis.

Primary image analysis

If correct parameter values are given, moving the cursor over the *Data Image* will give the qx-, qy-, and qz-component of the scattering vector in the group box at the upper left of the *Data Image*. It also displays the azimuthal angle and the intensity of the pixel at the cursor position.

Further analysis is possible by checking the check boxes in the *Cuts* group box at the right of the *Data Image*. Selecting the *left/horiz*-box displays a horizontal line, along which the intensity is taken and displayed in the upper image (*Analysis Image*). By changing the *tilt* angle below the *Cuts* group box, the intensity along lines with a finite angle with respect to the horizontal can be viewed. This is of interest, if lines and peaks are not exactly horizontal or vertical to the detector axis. By selecting *left/vert* or *left/circle*, the intensity along vertical lines and circular lines can be viewed as well. Also tilt angles can be chosen for these options.

Note that it is possible to draw simultaneous horizontal and vertical cuts for the *Data Image* (left image) as well as the *Model Image* (right image). For this, tick for images both the *horiz* and *vert* boxes. One can then move this “cross” simultaneously over both images. To get rid of a section line or circle, un-tick the corresponding box in the *Cuts* group box, then click on the image.

Cuts can be stored by clicking on the cuts and selecting *Save* → *Save left horiz data*, *Save* → *Save left vert data*, or *Save* → *Save left circle data* from the main menu. The file names should have the extension *.csv (Excel format).

The most recent of the selected horizontal, vertical and circular cuts can be displayed in the upper image by selecting *Plot* → *left horiz data*, *Plot* → *left vert data*, or *Plot* → *left circle data* from the main menu.

Note: The intensity distribution over a circle is particularly sensitive to the selection of the beam position. If the intensity distribution appears to be regular in the scattering pattern, but has large deviations in the display in the *Analysis Image*, then the beam position may be wrong and may require a further refinement.

Zoom in/out

To analyse the central part of the scattering pattern in more detail, select *Zoom* → *Zoom in* from the main menu. It displays the central quarter of the image around the beam. Horizontal, vertical and azimuthal (circular) cuts can be done as described above. To go back to the total image, select *Zoom* → *Zoom out* from the main menu.

Replot image

By selecting *Replot Image* from the main menu, the *Data Image* will be replotted. This is often done automatically, e.g. upon changing the color map or lin/log-scale. Replotting is necessary e.g. after changing the min/max-values or after displaying cuts as white lines in the image.

Masking

For averaging over selected areas of the image, it is often necessary to mask defective pixel areas or the shadow area of the beam stop. Masking can be done by selecting *Mask* → *Generate Mask* from the main menu. By clicking on the *Data Image* you sequentially specify the corners of the polygon whose interior represents the mask. The polygon is displayed with white lines. If the drawn polygon is acceptable, click *Mask* → *Accept mask* in the main menu. Then further masks can be generated. The masked pixels can be viewed by selecting *Mask* → *Show mask* from the main menu. If a drawn polygon is unacceptable, click on the RESET button in the *Mask* group box at the lower right of the *Data Image*. The generated masks can be saved by selecting *Save* → *Save Mask* from the main menu. They should have the extension *.msk. If mask files have been stored, they can be loaded by selecting *Mask* → *Load mask* from the main menu. After loading, the masked pixels can be displayed by *Mask* → *Show mask*. Further masks can be generated and stored together with the loaded masks.

In addition, pixels with values smaller than a certain minimum cut-off value can be masked by specifying this value in the *Mask* group box. Also, pixels with values larger than a certain cut-off value will be ignored, if this value is specified in the *Mask* group box.

All masked areas are ignored for the radial and sectorial averages.

Radial Averaging

Radial averages, e.g. averages over the azimuthal angle to give the intensity as a function of q , can be obtained by selecting *Average* in the main menu. One option is to average the whole image. The obtained scattering curve is displayed in the *Analysis Image*. It can be stored by selecting *Save* → *Save radial average* in the main menu. The filename has to have the extension *.csv as indicated by the filter in the save dialog. The most recent radial average can be replotted in the upper image by selecting *Plot* → *Plot radial average* in the main menu. Masked areas are not taken into account for averaging.

Often one likes to average just a particular sector of the image. This can be done by selecting *Average* → *define sector* from the main menu. The *Data Image* is then displayed in a larger format for higher accuracy. A green and red line are drawn from the beam center to the outer periphery of the scattering pattern. The part of the scattering pattern between the two lines will be averaged. This part corresponds to the part when going from the green to the red line in the counter-clockwise direction. The angle of the lines can be changed by clicking on the respective line, drag it to the desired position, and click once more to leave it at this position. The angular range to be considered for averaging is indicated by the black sector in the center

of the image. If the sector is appropriately chosen, select *Average* → *Accept sector* from the main menu. The sector average is calculated by selecting *Average* → *Average sector* from the main menu. Masked areas are not taken into account for averaging. The respective scattering curve is displayed in the *Analysis Image*. It can be stored by selecting *Save* → *Save sector average* in the main menu. The filename has to have the extension *.csv as indicated by the filter in the save dialog. The most recent sector average can be replotted in the upper image by selecting *Plot* → *Plot sector average* in the main menu.

Model calculations

Scatter allows one to calculate scattering patterns for the most common ordered structures. It can in particular calculate scattering patterns of anisotropic and oriented structures. Just as in the isotropic case, the Crystal Lattice is defined in the green *Crystal lattice* group box and the Particle shape as well as its interior structure in the blue *Particle* group box. Further the intensity and a flat background can be specified in the *IO and Background* group box.

For oriented structures an

- azimuthal domain size

which relates to the azimuthal peak width needs to be specified. Further, many structures occur in the twinned form (fcc, bcc, hcp). If twinned, the check box *twinned* will be checked, and the

- fraction of each twin needs further to be entered.

For anisotropic particles like cylinders and disks, their main axis (cylinder axis, disk normal) may be oriented in a certain direction with some angular distribution around this direction. For them in the *Orientalional Distribution Function* group box

- an orientational distribution function needs to be specified together with
- a parameter *dbeta*, which is very small (<10) or zero for perfect alignment, or large (20 – 50) for intermediate alignment to very large (>>100) for nearly isotropic orientations.

Further for oriented samples one needs to specify the orientation of the lattice structure with respect to the beam. This is done in the *Calculation* group box. One needs to specify

- the Miller indices [hkil] of the direction in the reciprocal lattice that is parallel to the beam.

To determine the crystal orientation with respect to the beam is usually a first task for a two-dimensional data analysis. One can enter the hkl-indices, e.g. 1, 1, 1 for the [111]-direction in an fcc-lattice in the blue edit fields. For hexagonal systems an additional index *i* (here in grey) is often given. It needs not be entered, since it will be calculated from the main Miller indices. Next

- the Miller indices of the directions in reciprocal space that are parallel to the qx- and qy-axis of the scattering pattern need to be specified.

Their Miller indices are entered in the edit fields below *x* (for qx) and *y* for (qy) on the right side of the blue edit fields. If these directions are not known, one can let the program select directions by clicking the radio button *none* in the group box *Fix axis*. If at least one direction is known, it can be entered either in *x*- or *y*- and the corresponding radio button *x* and *y* have to be selected in the *fix axis* group box. As an example, directions parallel to the *x*-, *y*-, and *z*-axis are [100], [010], and [001] for cubic unit cells, and [2-10], [010], and [001] for hexagonal unit cells.

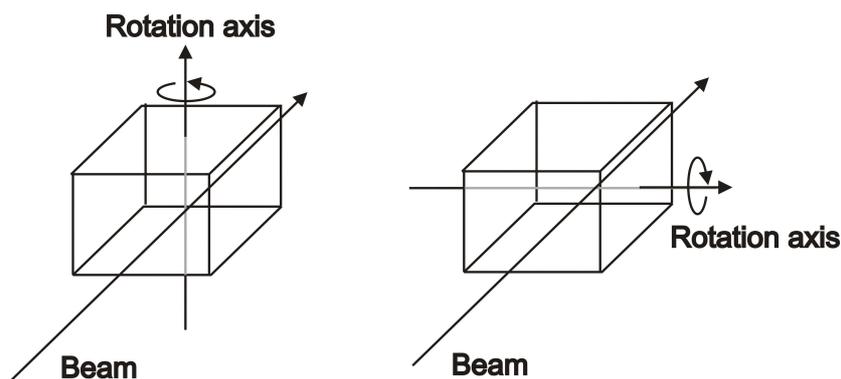
Rotations

Some experimental setups allow one to rotate the sample to collect the scattering patterns corresponding to different projections of the lattice. For modelling calculations the unit vector corresponding to the $[hkl]$ direction which has been specified in the blue edit fields can be rotated around an arbitrary axis specified by

- its Cartesian components in the *rot_axis* edit fields by
- an angle (in degrees) that is specified in the *rotate* edit field.

This will yield a $[hkl]$ -direction that is specified in the *n(rot)* edit field. In practice the sample is usually rotated (a) around a vertical axis (Fig. 2a), (b) around a horizontal axis (Fig. 2b), or (c) around an axis that is parallel to the beam (Fig. 2c).

- (a) In this case the rotation axis is parallel to the qy -axis and the cartesian coordinates of this axis are entered in the *rot_axis* edit fields. Since the directions of the qy -axis will be the same for all rotated patterns, one will fix the qy -axis for this series of patterns
- (b) Here the rotation axis is parallel to the qx -axis and the cartesian coordinates of this axis are entered in the *rot_axis* edit fields. Since the directions of the qx -axis will be the same for all rotated patterns, one will fix the qx -axis for this series of patterns
- (c) This rotation corresponds to tilting the scattering pattern. Here a rotation axis needs not be specified. Only the tilt angle has to entered in the tilt edit field.



Number of quadrants

Next the number of calculated quadrants of the scattering pattern needs to be specified by clicking on one of the radio buttons in the *quadrants* group box. Most scattering patterns have point symmetry (Friedels law) so that it is sufficient to calculate just 2 quadrants of the scattering pattern. In this case 2 is selected. The other half is generated by inversion. This saves time required for the calculation of the pattern. Often scattering patterns have four-fold symmetry. Then it is sufficient to calculate just 1 quadrant. Just to be sure, one can also calculate all four quadrants, which then takes longer for the calculation of a pattern.

Centering

Scattering patterns can be calculated either with their center in the middle of the image, or with their center at the position of the beam of the corresponding experimental scattering pattern that is displayed in the *Data Image*. If the center should be in the middle, then select

the radio button *mid point* in the *Center* group box. This is an option for just modelling scattering patterns without quantitative comparisons to specific experimental data. For quantitative comparisons with the data in the *Data Image*, the radio button *beam* is selected in the *Center* group box. If data files are loaded, *beam* is automatically selected.

For first analysis, the whole scattering patterns usually have to be calculated. For this the radio button *full image* is selected. For refinement of model parameters at a later stage it is often sufficient to calculate just slices or cuts of the whole pattern and to compare them to the experimental cuts. This will later be done by selecting the *slice* radio button.

The calculation is performed up to a maximum q-value that is specified in the *qmax* group box. This can be either preset by selecting the radio button *preset* and entering the desired value below. For quantitative comparisons with the data in the *Data Image*, the radio button *data* is selected in the *qmax* group box. Then the image will be calculated exactly within the q-range of the experimental data. If data files are loaded, *data* is automatically selected.

Then the number of gridpoints of the calculation needs to be specified. These are the gridpoints within one quadrant of the calculated scattering pattern. A number of gridpoints 20 will calculate a quadrant of 20x20 pixels yielding a 40x40 pixel image. For a calculation of 2 quadrants this gives a crude first image without a lengthy calculation and is often sufficient to give a first idea of the scattering pattern. The maximum number of gridpoints is 150.

Modelling – first phase / Find Lattice

From here the first part of the modelling usually starts. One needs to find out the type of crystal lattice, its orientation and adjust the unit cell dimension and particle dimensions so that the positions of the calculated peaks resemble the position of the peaks in the experimental pattern. This often takes time. As a help, choose a possible crystal lattice from the *Crystal Lattice* group box and specify a possible hkl-value for the beam = qz-direction displayed in light blue. By selecting *FindLattice* → *Search* from the main menu the *Data Image* is displayed in larger size and the set of Debye-Scherrer rings and Bragg-reflections corresponding to the selected crystal lattice and beam direction is displayed. Reflections in green are allowed reflections, reflections in yellow and red are forbidden, but can sometimes occur if the sample consists of domains with different orientations (texture) or if the domains are small. Moving with the cursor over the *Data Image* will shift the position of the Debye-Scherrer rings and Bragg-reflections. If there is good agreement between the positions of the reflections, click on the cursor position. Then the corresponding value of the unit cell size and tilt angle are stored for a subsequent calculation. If no agreement can be found select *FindLattice* → *Done* and check for other crystal lattices and beam directions.

By selecting *Calculate* from the main menu the calculated image is displayed in the lower right image (*Model Image*). Moving the cursor over the *Model Image* will display the q-values, the azimuthal angle and the calculated intensity *I_{th}* in the group box on the left side of the *Model Image*. It will also index the peaks at the cursor position and give its Miller indices below the intensity *I_{th}*. If a reflection is allowed then a green bar will appear below the Miller indices of the peak. Forbidden peaks can sometimes be visible because of their large peak width. These peaks will be indexed together with a yellow or a red bar. The center of these peaks will have some finite distance from the Ewald plane. This distance is given below the bar. For allowed reflections this distance is zero. Reflections with large distances are indicated by a red bar and are usually not or only slightly visible.

Often the *Model Image* appears just to be rotated with respect to the *Data Image* by some angle. By entering a value for the respective *tilt-angle* in the *Calculation* group box, a rotated image will be calculated. This requires to set the number of calculated quadrants to 4.

For further help and visualization the projection of the structure in real space is calculated by selecting *Projection* in the main menu. The projection is displayed in a small image right above the *Model Image*. The projection corresponds to an image that would be obtained by transmission electron microscopy. It is the relevant information in real space that corresponds to the calculated scattering pattern (According to the projection theorem of Fourier transforms, a projection in real space corresponds to the scattering pattern in reciprocal space). The projection can be stored by selecting *Save* → *projection* from the main menu. The image is stored as a bitmap. The filename has to have the extension *.bmp as indicated by the filter in the save dialog.

Modelling – second phase

If the position of the reflections of the *Model Image* and the *Data Image* are in reasonable agreement, one can proceed with the next stage of the data analysis. For this the *Model Image* has to be calculated with at least 80 gridpoints. By selecting *left/horiz* and *right/horiz* in the *Cuts* group box, a white horizontal line is displayed in the *Model Image* and in the *Data Image*. The intensity along these lines is displayed in the *Analysis Image*. For the *Model Image* it is displayed in blue, for the *Data Image* in red. One can then adjust the model parameters, perform a new calculation and compare the new calculated values with the experimental values. By selecting *left/vert* and *right/vert* or *left/circle* and *right/circle* also vertical and circular cuts can be compared. By simultaneously selecting the horizontal and vertical lines in each Image, peak positions in both images can be compared.

Within the course of the analysis, values of many model parameters will have to be adjusted, requiring every time a calculation of a scattering pattern, which can be quite time consuming. To proceed further it is possible just to calculate the slice of the *Model Image* that corresponds to the horizontal, vertical or circular line displayed in the *Data Image*. This is done by selecting *slice* in the *Calculation* group box. When e.g. *left/horiz* is selected, the intensity distribution along the horizontal indicated by the white line is displayed in the *Analysis Image*. To calculate the corresponding slice hit CTRL C to start the calculation without moving the cursor. This is much faster compared to the calculation of the whole image and the optimization of the parameter values proceeds faster. One can similarly proceed for vertical and circular lines in the *Data Image*. Also the tilt angle for the lines can be adjusted. Once and a while the calculation of the whole pattern is necessary, because for some parameters the agreement may become better on the horizontal line, but may become poorer along vertical and circular lines. The calculated slice can be stored by selecting *Save* → *Save slice calculation* in the main menu. The most recent slice can be displayed in the upper image by selecting *Plot* → *slice calculation* in the main menu.

Modelling – third phase

At a stage, where the *Model Image* has reached good agreement with the *Data Image*, further optimization of model parameters can become quite tedious, because many time-consuming small adjustments have to be made. This is a stage where an automated fitting procedure can

optimize the parameters further. In principle, a whole 2-dimensional *Model Image* can be fitted to the *Data Image*. This would be very time-consuming and practically not feasible. In addition, as the information on the *Data Image* is reduced to only a few structural parameters, the information contained in the *Data Image* is highly redundant. It is much more practical to select a few lines or circles in the *Data Image* from which the structural parameters can be derived. These are e.g. lines through characteristic peaks, oscillations and other features of the scattering pattern. The intensity along these lines can then be fitted to the model.

To select such lines/circles, select *FileSeries* → *Select Lines/Circles Set* from the main menu. Now select e.g. by choosing *left/horiz* a horizontal line and move it to the desired position and click on it. The intensity along this line is now stored. Then select another horizontal, vertical or circular line, move it to the appropriate position and click on it. Usually, 1 – 3 lines/circles are sufficient for a first fitting analysis. At maximum ten lines/circles can be stored. The lines/circles set can then be stored in a file by selecting *FileSeries* → *Store Lines/Circles Set for Fitting* or by selecting *Save* → *Save cuts for fit* in the main menu. The filename has to have the extension *.csw as indicated by the filter in the save dialog. The fitting will be performed in the *ID-Crystal* program.

The parameter values that had been optimized can be saved in a parameter file. This is done by selecting *Parameter* → *Save parameter file* in the main menu. The filename has to have the extension *.par as indicated by the filter in the save dialog. In *ID-Crystal* the data can be loaded, modelled and fitted.

If the agreement between the *Model Image* and the *Data Image* is sufficiently good, a direct comparison can be made by merging parts of the *Model Image* into the *Data Image*. If e.g. you want to copy the right upper quadrant of the *Model Image* into the *Data Image*, then select *MergePlots* → *upper right quadrant* from the main menu. This allows for a good quantitative comparison of both images. The *Data Image* can be stored by selecting *Save* → *DataImage* from the main menu. The file is a bitmap and has to have the extension *.bmp as indicated by the filter in the save dialog. The *Model Image* can be stored by selecting *Save* → *Calculated Image* from the main menu. Also this file is a bitmap and needs the extension *.bmp.

Data Series

Often one has a large number of *Data Images* that were collected under the same experimental settings, i.e. beam position, sample detector distance. Then it is desirable to consecutively analyse these data automatically. Scatter allows one to calculate radial averages (whole image or sector) and display and store cuts for further analysis and fitting. As described above, this can be done for file series with consecutive numbering or for all files stored in a common folder.

To just quickly view a series of files select *FileSeries* → *Select Series Specification*. Then the *Series File Format* group box appears on the upper right of the *Analysis Image*. Select the positions in the file name that contain the numbering. Then press either *next* or *previous* button in the *View File Series* group box on the upper left of the *Analysis Image* to view the previous or next file in a series of files.

Series averaging

First one of the files is loaded and it is made sure that the parameters in the *DataInfo* group box like beam position, detector distance etc. are correct. For averaging the full image of a file series with consecutive number, select *Average* → *Select Series Specification* from the main menu. Then the *Series File Format* group box appears on the upper right of the *Analysis Image*. Select the positions in the file name that contain the numbering. Then select *Average* → *ImageSeries* from the main menu. Then click on the first file and the last file to be averaged. Then, as can be seen on the progress bar (moves three times each file) each file is loaded, displayed, averaged and then stored with the filename and the filename with the name/extension *_i.csv. If all files in a folder should be averaged, select *Average* → *ImageFolder* from the main menu and select the folder containing the files. Then all files in the folder are averaged and the resulting scattering curves stored as *.csv files.

For sector averages define the sector as described above. Then select *Average* → *Select Series Specification* from the main menu to specify the file numbering. Then the *Series File Format* group box appears on the upper right of the upper image. Select the positions in the file name that contain the numbering. Then select *Average* → *Sector Series* from the main menu. Then click on the first file and the last file to be averaged. Then, as can be seen on the track bar (moves three times each file) each file is loaded, displayed, averaged and then stored with the filename and the filename with extension *_s.csv. If all files in a folder should be averaged, select *Average* → *SectorFolder* from the main menu and select the folder containing the files. Then all files in the folder are averaged and the resulting scattering curves stored as *_s.csv files.

Line/circle sets and file series

To store line/circle sets of *Data Images* select *FileSeries* → *Select Series Specification* from the main menu to specify the file numbering of the series. Then select *FileSeries* → *Select Lines/Circles Set* from the main menu. Then by e.g. using *left/horiz*, moving the horizontal line with the cursor and selecting by clicking, select a number of lines (horizontal, vertical, circular) whose intensity should be stored for further modelling and fitting. Then select *FileSeries* → *Store Line/Circle Set Series for Fitting* from the main menu. Then select the first and last file from which the line/circle sets should be extracted. Then, as can be seen from the progress bar (moves two times each file) each file is loaded and displayed, the line/circle sets are extracted, and the files are stored as *_c.csw files. This can be similarly applied for a folder by selecting *FileSeries* → *Store Line/Circle Set Folder for Fitting*. The *.csw file series can then be series fitted in 1D-crystal, so that an automated analysis of large series of anisotropic data images is possible.

To just view a single line/circle of a file series select *FileSeries* → *Select Series Specification* from the main menu to specify the file numbering of the series. Then click *FileSeries* → *Select Lines/Circles Set* and choose *left/horiz*, *left/vert* or *left/circle* to position a line or circle on the *Data Image* and click on it. Further select *overlay* or *colormap* from the radio buttons in the *Series File Format* group box. Then select *FileSeries* → *View Single Line/Circle Series* to view the data either as overlaid data point series (*overlay*) or as colorbands (*colormap*) in the *Analysis Image*.

To store a line/circle of a file series for display (not fitting), specify the file numbering and select the line/circle as described above. Then select *FileSeries* → *Store Single Line/Circle*

Series for Display and select the first and last file from which the line/circle sets should be extracted. Then the lines/circles are extracted from the files and stored as *_c.csv files. To select the files from a folder, click *FileSeries* → *Store Single Line/Circle Folder for Display*.

Note: In all cases that files from a folder are chosen it should be checked that the folder only contains files of the same file type.

After storing or in case of inappropriate line/circle selection select *FileSeries* → *DONE* to reset the line/circle set to zero.

Print

A screenshot can be printed by selecting *Print* from the main menu. This is useful to have a documentation of current parameter settings, data and model images.

Example

The default values in boxes *Crystal Lattice* and *Particle* correspond to an image obtained at the ESRF on beam-line ID02 (file *sc2304_0_0829ccd*). For this pattern, the *Crystal Lattice* is a *FCC (Fm3m)*, the *Peak Shape* is *Gaussian*, the size of the *unit cell* is 79 nm (it's a cubic Bravais lattice), the radial domain size (*rad. domain*) which is inversely proportional to the radial peak width, is 400 nm, the azimuthal domain size (*azi. domain*) which is inversely proportional to the azimuthal peak width, is 180 nm, and the average *displacement* from the lattice as calculated from the Debye-Waller factor, is 2 nm. The field *max. hkl: 5* indicates that we take into account peaks up to the fifth order.

In the *Particle* box, we consider that the *Particle Shape* is a *Sphere* with a *radius* of 13 nm, and that the *Particle Interior Structure* is *homogeneous*. The polydispersity of the spheres *sigma(R)* is 0.05 (this means 5% relative standard deviation). Note that the set of parameters available in the *Particle* box depends on the particle shape and internal structure. For instance, a homogeneous cylinder is characterized also by a *length* and a *sigma(L)*.

Back to our example, make sure that $h=1$, $k=1$, $l=1$ in box *Calculation*. This corresponds to the (1, 1, 1) direction of the FCC lattice. The *fix axis* is x and the rotation axis (*rot_axis*) corresponds to the (1, 1, -2) direction. The calculation can be done for one, two, or four quadrants. In our case, one is enough because of the symmetry of the structure. The *Center* of the diffraction pattern corresponds to the indicated *beam* position, rather than to the geometrical center of the picture.

Click on *Calculate* (shortcut *Ctrl-C*) to start calculating the scattering pattern. A progress bar follows the advancement of the computation. The simulated pattern is then displayed in the lower right image. For a more detailed calculation, one can increase the number of *gridpoints* in box *Calculation*. This will take some time.

You can interrupt the calculation at any time by pressing *ESC*.