Overview of the reflectometer instrument

1 The instrument

This reflectometer instrument is a virtual instrument, since it is simulated rather than actually running in the real world. However, in most practical purposes, you can still think of it as a real instrument, with different components and samples.

1.1 Overview of the instrument

The instrument simply consists of a source (of which the wavelength bandwidth can be changed), two slits (of which the widths and position can be changed), a sample (which can be altered in different ways, be translated and rotated) and a detector (which can be rotated around the sample position). The distances between the different components can be changed by the user. An overview of the instrument, along with some of the simulation-parameters that can be set before run-time, is shown in figure 1.
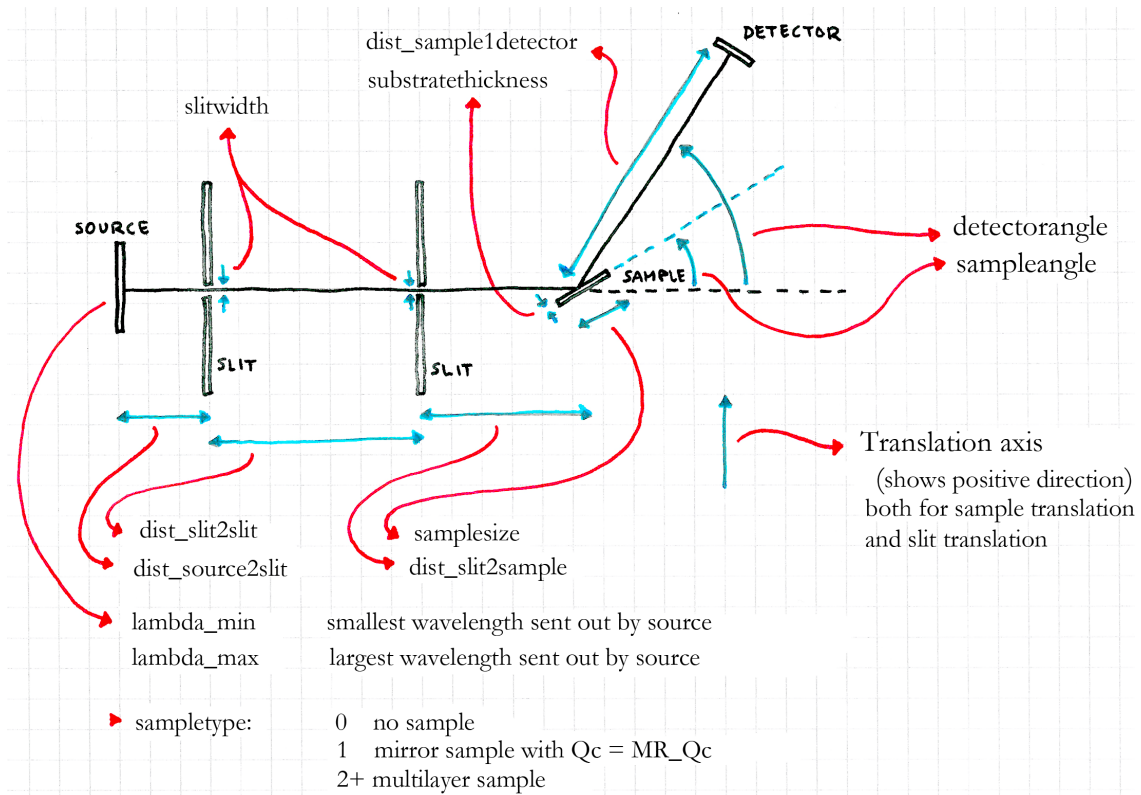
Figure 1: Top-view of the instrument with some of the instrument parameters drawn in.

1.2 Parameters

The simulation has a large number of parameters, which all change the instrument somehow. These are listed below. They all have default values, which should work together – such that a simulation run using these values should actually yield a meaningful result. So when in doubt, simply leave the default values in.

The most important ones (the ones to be changed by the students during the exercises) are written in bold. Note that the translation axis has been shown in figure 1, in order to know in which direction is positive!

Parameter	Unit	Default	Description
lambda_min	Å	5.3	**Minimum wavelength from source**
lambda_max	Å	5.45	**Maximum wavelength from source**
slittranslation	m	0	**Translation of slit (horizontal)**
sampletranslation	m	0	**Sample translation (horizontal)**
slitwidth	m	0.01	Width of slit pinholes
slitheight	m	0.05	Height of slit pinholes
dist_source2slit	m	1	Distance between source and first slit
dist_slit2slit	m	3.2	Distance between slits
dist_slit2sample	m	0.18	Distance between second slit and sample
dist_sample2detector	m	2	**Distance between sample and detector**
sampletype	1	1	**Sample type: 0 none, 1 mirror, 2+ multilayer**
samplesize	m	0.15	Side-length of the (quadratic) sample plate
substratethickness	m	0.003	Thickness of the substrate
MR_Qc	Å	0.15	**Mirror: Critical Q-vector length**
sampleangle	deg	2.5	**Rotation angle of sample (θ)**
detectorangle	deg	5	**Rotation angle of detector (2θ)**

Note that the sampletype parameter is special: It changes the sample. When set to "0", the sample is simply removed. When set to "1", the sample is a mirror, which is to be used for the alignment exercises explained later. When set to a value above 1, the sample is a special sample following some actual real samples, as follows: 2, d54DMPC-D2O; 3, d54DMPC-H2O; 4, hDMPC-D2O; 5, hDMPC-H2O; 6, silicon-D2O; 7, silicon-H2O.

1.3 The live-simulation tool

The simulations are run by the simulation package McStas (http://mcstas.org). However, in order to not have to install and run it on your own computer, a web-frontend has been made, such that the simulations can instead be run from a web browser.

After logging in to the live simulation page (links and logins will be given at the exercises), you will have to choose the instrument called "reflectometer". Now you see a list of the simulation parameters, each with the default values already filled in.

In the bottom, you will also see a box with name "Rays (ncount)". This is the number of neutron rays that you want to simulate, and is already filled in with the default value, one million. This can be highered if your statistics is bad – but note that a higher number of rays will of course take longer time to simulate!

You will also see a box with name "Scan num-points". By default, this is filled with a "1", and the simulation runs once with the parameters that has been set. If instead you want to do a scan over some range of one (or several) of the parameters, you can here set how many points you want to simulate.

1.3.1 Getting the data out

Once you've run a scan, a pop-up window will open[1], slowly updating with all the simulated data shown in plots. The first 9 plots are different detectors along the instrument (position-sensitive detectors, divergence distribution detectors and wavelength distribution detectors – the names in the top of each plot should show where the detector is positioned). The most important detector is the last one (this is the one showed as the detector in figure 1).

You can press "l" on your keyboard to get the intensities on a logarithmic scale. This often gives a better view of what actually happens, especially when doing $\theta/2\theta$ scans (explained below).

You can click each of the images once, to get a higher resolution image. If you click this larger image, you get to the datafile behind the plot (simply use "back" in your browser to get back).

1.3.2 Scanning

To do a scan over a variable, you simply put in the start and the end value with a comma between them, instead of a single value. The number of scan points set in the "Scan num-points" then decide the number of values inbetween these two values (with a linear interpolation).

In order to do a $\theta/2\theta$ scan (where the sample is at one angle, and the detector is at twice this angle – and they follow each other over a scan), you need to tell the simulation the start and end points for both of the parameters (here `sampleangle` and `detectorangle`). Say you want to scan the sample from 0 to 6 degrees (and hence the detector from 0 to 12 degrees). Then you put in "0,6" in the box for `sampleangle`, and "0,12" in the box for `detectorangle`. Then both the parameters will get higher in a linear way, following the set number of scan points, such that the detector angle is always the double of the sample angle.

When you've done a scan, only a single image is shown in the pop-up window. This image contains plots of the intensities as functions of the scan-points, for each of the detectors. Here you will normally only look at the last of the detectors. This image can also be clicked, in order to get to a larger version, and clicked again to get the datafile.

In the datafile, the scan-variables are listed as the first column(s), while the intensities on the different detectors (and the error on these numbers) are in the next columns (just above all the columns, a header line actually writes all the column names). So, the next-last and last columns are the intensity on the detector, and the error on this number. These can be imported to excel, or similar, by copy-pasting the text.

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[1]If you instead get errors, your browser might be blocking pop-ups. Allow pop-ups for the site, and then reload it and log in again.

2 Alignment of sample

This section goes through a method to make sure that the instrument is aligned properly. Try to follow the different steps, and make the mentioned scans yourself. See if you get to the same conclusions, or if your instrument setup is mis-aligned!

2.1 Detector angle

Here we use no sample. In order to make sure that the detector angle is actually zero degrees when the parameter `detectorangle` is zero, a scan is done of `detectorangle` around 0.

This scan can be seen in figure 2, and show a centered peak. This is also a measurement of the direct beam, which can be used for normalization later.

2.2 Sample translation

In this we use a mirror sample. Here we set the detector angle at zero degrees, and translate the sample along the translation axis as shown in the overview figure (figure 1).

A scan is done of `sampletranslation` around 0. This scan can be seen in figure 3, and show a trapezoidal shape. To find where the sample should actually be positioned, one finds the centerpoint of the trapez (can be done both by looking at the top or the bottom part), and subtracts half the width of the sample (which is the width of one of the sloping parts of the curve). Setting the sample at this position, the top part of the sample (the actual mirror) is centered in the beam.
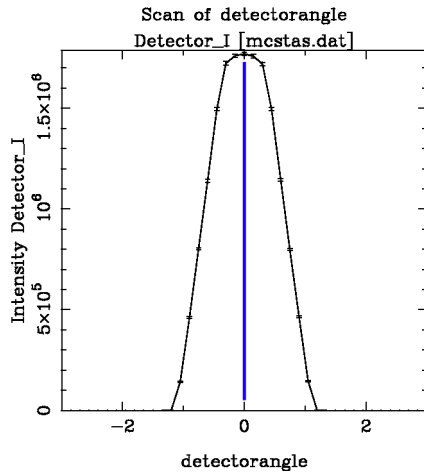

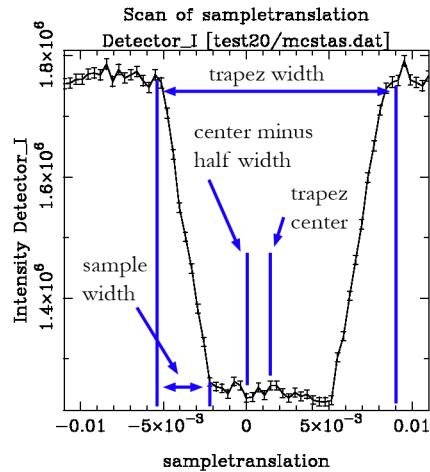Figure 2: Scan of detector angle when there is no sample.

Figure 3: Scan of sample translation with a mirror sample.

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2.3   Sample rotation

In this we use a mirror sample. Again we keep the detector angle at zero degrees, and now rotate the sample around the center position (as found above).

A scan is done of `sampleangle` around 0. The scan can be seen in figure 4, and show a nice centered peak. It is, however, a bit skewed to the positive angles. This is because of the mirror, which reflect some of the neutrons towards the detector at positive angles, but not as much at negative angles (where the neutrons are instead absorbed by the substrate below the mirror).
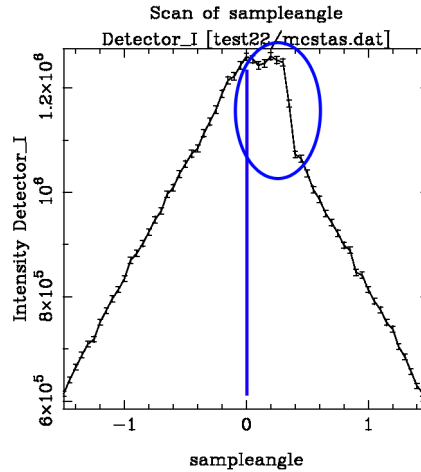

Figure 4: Scan of sample angle with a mirror sample.

Instead of having the detector at zero degrees when doing this scan, it is possible to do a specular scan instead (then we won't have to worry so much about the direct beam): Placing the detector at a certain angle (less than two times the critical angle of the mirror), and then scan the sample angle around the half-value. Such a scan can be seen in figure 5, where the detector is at an angle of 5 degrees. The same scan done with a larger sample-detector distance is shown in figure 6, showing the resolution change.
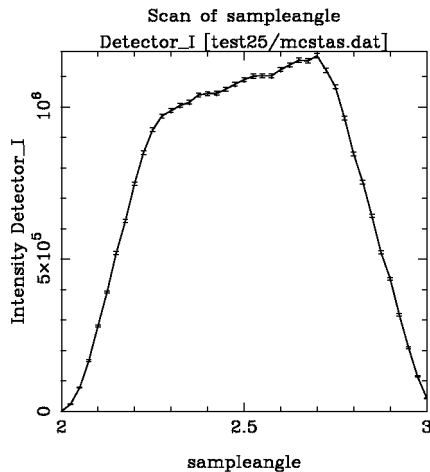

Figure 5: Scan of sample angle with a mirror sample, around a specular refraction. Detector at 1 m.
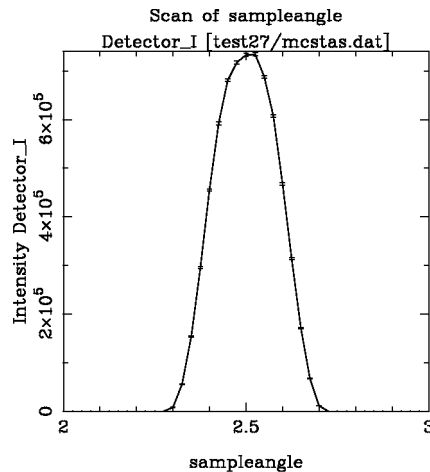

Figure 6: Scan of sample angle with a mirror sample, around a specular refraction. Detector at 3.2 m.

2.4 Slit translation

In this we use a mirror sample. Here we want to do a footprint scan, keeping the sample and detector at some fixed specular reflection, and scanning the slit position along the translation axis.

A scan is done over `slittranslation` around 0. The scan can be seen in figure 7, showing a nice centered peak.
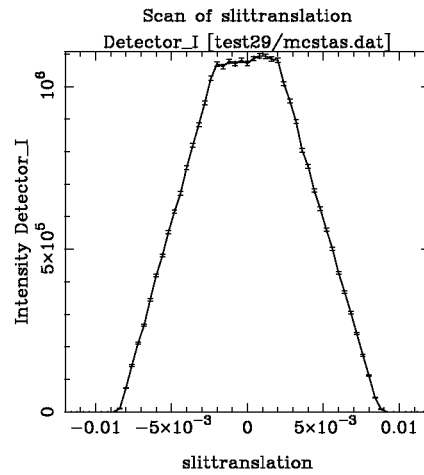

Figure 7: Scan of slit translation.

3 Different samples

3.1 Mirror

The mirror sample is fairly simple, and primarily used for the alignments shown above. A full scan of a reflection curve can be seen in figure 8. Note the direct beam for small angles, and the fall in intensity when going to smaller angles (before hitting the direct beam). We have a $\sin\theta$ dependence on how much sample is hit by the beam! (Try correcting for this when importing and plotting the data in excel.)

The critical angle is also seen nicely, and it can be changed by changing the Q_c value in the sample (the `MR_Qc` parameter).

3.2 Multilayer

A simple multilayer scan can be seen in figure 9. Once again we see the direct beam, but it's harder to see the $\sin\theta$ dependence.
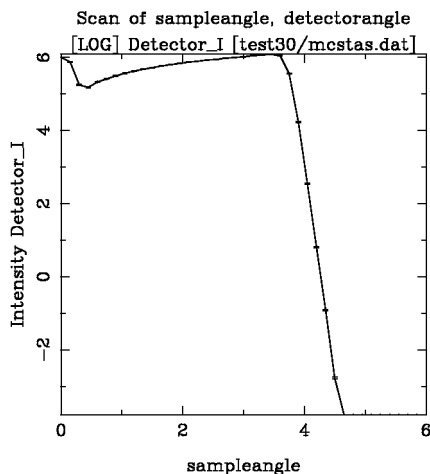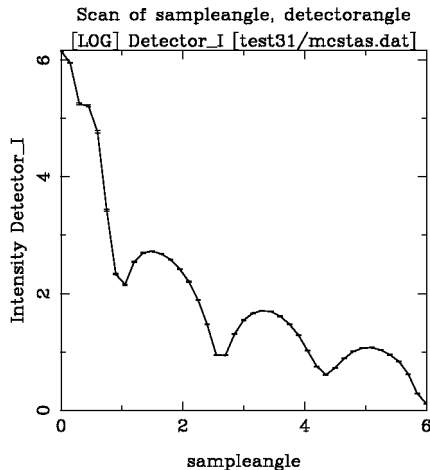

Figure 8: θ-2θ scan for a mirror sample.

Figure 9: θ-2θ scan for a multilayer sample.

The multilayer sample used here has the following characteristics (as made from the `http://alanine.usc.es/sangra/` page):

	SLD [10^{-6} Å^2]	Thickness [Å]	Roughness [Å]
Solvent/air	0	—	—
Layer 1	5	30	0
Layer 2	5	30	0
Layer 3	5	30	0
Substrate	10	—	0
Background: 1×10^{-6}		Scaling factor: 1	

This multilayer is, however, not part of the simulation given in the exercises. Instead you have six different choices of samples to work with, and should try looking at them all – comparing the ones with H_2O and D_2O.

Try also to calculate the angle axis into a q-axis instead, using the wavelength that the simulation is using, along with $q = 2k\sin\theta$ (and $k = 2\pi/\lambda$).