Overview of the reflectometer instrument

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.

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. This instrument can only work in monochromatic mode.
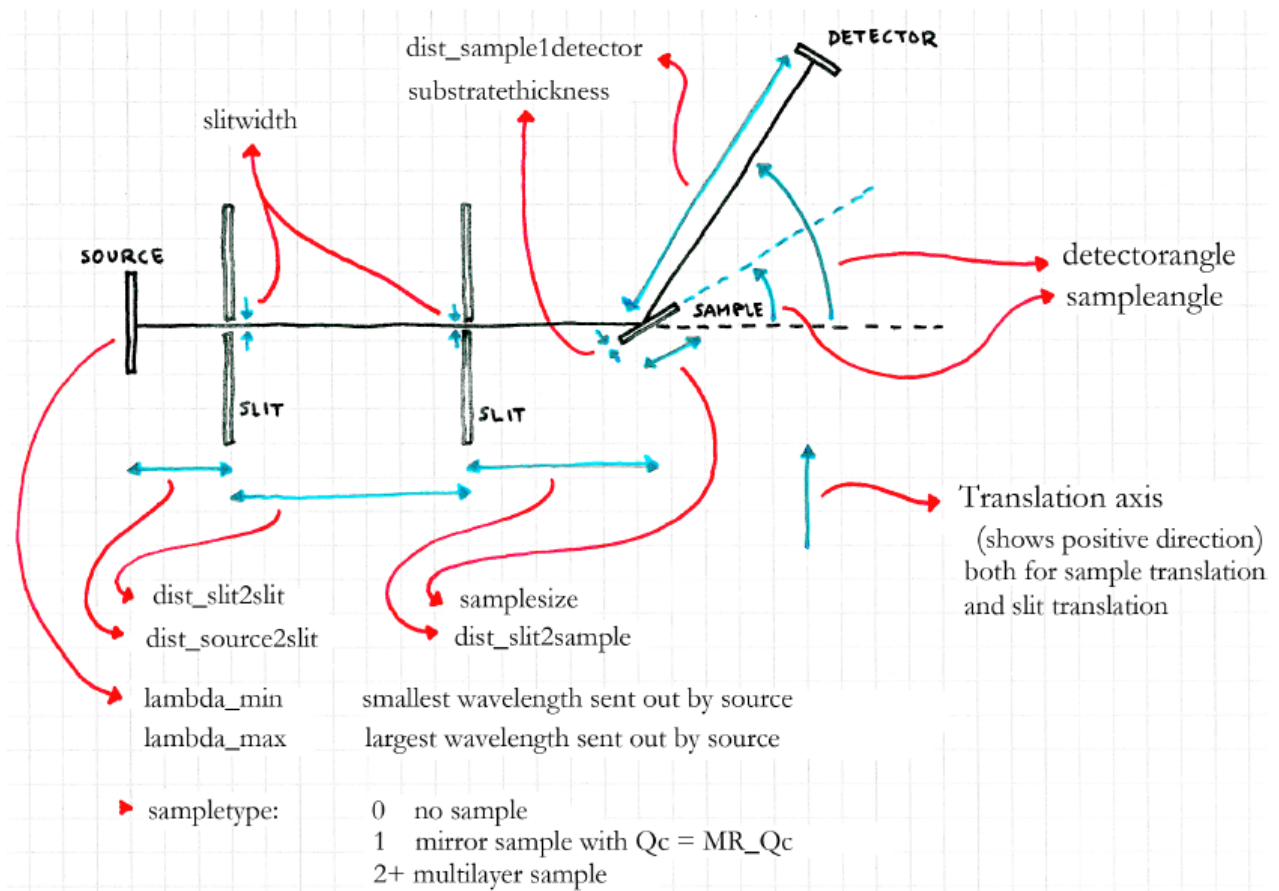

Figure 1: Top-view of the instrument with some of the instrument parameters drawn in.

Parameters

The simulation has a large number of parameters, which all change the instrument somehow. These are listed below. The table below shows the default values you should use to get started in your simulation. 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	0.001	Width of slit pinholes
slitheight	m	0.002	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. Also double check that the settings in the instrument file corresponds to the ones described in the table above.

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 (please check the values are correct, specially for the slit widths). 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 increased 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.

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=2thetha 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 data file behind the plot (simply use \back" in your browser to get back).

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 in between these two values (with a linear interpolation).
In order to do a theta=2theta 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 data file. In the data file, 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.

The exercise

Neutrons are reflected or refracted at an interface depending on the difference of the refractive index (or scattering length density) of the two media that form the interface. At small enough angles, no refraction occurs and this condition is known as total reflection.

1) Imagine that you are have the following three interfaces and you need to measure processes at them using neutron reflection:

1.1) D_2O against air
1.2) silica against D_2O
1.3) Au against air

Set the instrument so that you can cover the following Q range 0.5*Qc to 20*Qc, where Qc is the critical Q at which refraction starts to occur. In order to calculate the scattering length densities of the material please go to

http://www.ncnr.nist.gov/resources/sldcalc.html

2) Run a simulation with the settings you have calculated and verify the Q range was correct by obtaining the expected reflectivity curve. For this you off course will need to change the MQ_Qc and sampleangle/sampledetector in your parameter list accordingly to the system you are supposed to probe.

3) The data you obtain is not normalize. How can you normalize it?

4) Now let's double check that the settings for the slits were optimal for our sample. For this you will have to calculate the footprint of the neutron beam on your sample at the smallest angle of incidence.

5) By choosing sample 5 you will get a reflectivity curve of an unknown sample at the Si-D2O interface. Assuming it is some sort of soft matter sample (a surfactant for instance), calculate the approximate total thickness of the layer.