

Vitess sample exercise

Task 1: Powder sample reconstruction with fixed wavelength

Create an instrument comprising a constant source, a curved guide, a collimation system consisting of two slits followed by a powder sample and a detector. Reconstruct the powder spectrum using the eval_elast module. Why do the reconstructed peak intensities vary? Look up the help on the sample_powder module and figure out the main dependencies of the scattering probability. Try also varying the waveband range or the reference wavelength in the eval_elast module.

Details:

Source: A disc with 12 cm diameter emitting neutrons **between 1.98 and 2.02 Å**, 150 cm distance to the guide, **use at least 5e7 trajectories.**

Guide dimensions: 6x6 cm² cross section, length 20 m, curvature radius 1000 m.

Coatings:m=3

Slits: 1st slit: 2(width)x4(height) cm², 1 m away from the guide exit; 2nd slit: 1x4 cm² 3m away from the first slit

Sample: powder sample module, details see picture (input files provided):

Module 11 sample_powder

sample file SynE.pow Browse BrowseN Edit

Theta [deg] 80 dTheta [deg] 75 Phi [deg] 0

dPhi [deg] 3.5 repetitions 1 colour 1

incoherent scattering no

treat all neutrons no

Detector: cylindrical detector, details see picture:

Module 12 detector
General detector geometry

array (first or intermediated part)

geometry type usage

repetition detect color add color

phi [deg] theta [deg] distance [cm]

height [cm] width [cm] thickness [cm]

number of rows number of columns number of layers

hor. resolution [cm] vert. resolution [cm] resolution in x [cm]

efficiency modifier

lambda efficiency

absorber/convertor type

gas pressure [bar] or solid layer thickness [cm] gas temperature [K] or atom density (solid) [10^{27} 1/m³]

Evaluation for elastic scattering: eval_elast, details see picture (syn_info file provided):

Module 10 eval_elast

evaluation parameter

spectrum file AutoPlot

intensity file

info file

number of bins minimum [A, 1/A, deg] maximum [A, 1/A, deg]

increase to next bin[%] dead-spot [deg]

probability weight exclusive counts scattering axis of the sample

time of flight correct to distance

flight path [cm] sample-detector distance [cm] time offset [ms]

reference wavelength [A] time interval begin [ms] time interval end [ms]

Monitors: 2D position, 2D divergence in front of the first slit

Task 2: Powder sample reconstruction with variable wavelength

Use the instrument built in the previous task and add a pulse shaping disc chopper. The chopper is used to create a short pulse and thus encode the wavelength information in the time of flight of neutrons. The

eval_elast module should be switched from reconstruction using a reference wavelength to use the time of flight information. What is the correct distance to enter as flight path and sample-detector distance? Why do the reconstructed peak intensities vary much stronger now?

Details:

All as before, in addition:

Source: Change the window to 2x2 cm, **waveband 1 – 9 Å, time 0 to 4 ms**, use at least 5e7 trajectories.

Disc chopper: Location at 1.5 m away from the source, frequency: 15000 rpm, offset: -80°, distance to previous module: 0, number of eq. windows: 1, set zero time: **yes** (what happens if you change to “no”?), **input file**: disc radius 40 cm, vert. axle 33, hor aisle 0, window pos 140°, window height: 14 cm, window width 10° (check with the help file!).

Monitors: Wavelength monitor after chopper; wavelength, 2D lambda vs tof monitor after slits, 2D lambda vs divy monitor after detector.

Evaluation for elastic scattering: eval_elast, details see picture:

The screenshot shows the 'Module 14 eval_elast' configuration window. The parameters are as follows:

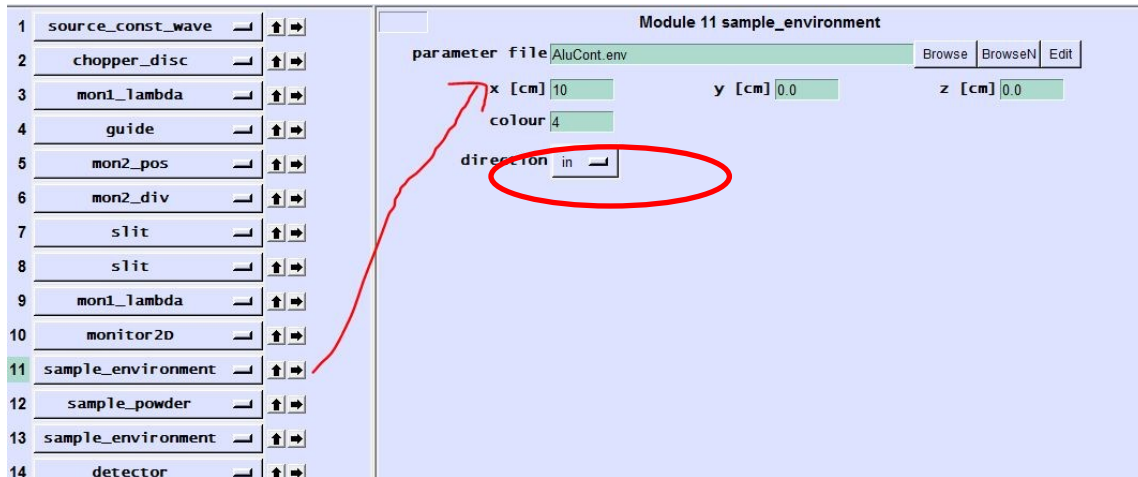
- evaluation parameter:** d-spacing [Å]
- spectrum file:** eval_syn_sample.eva (with Browse, BrowseN, Edit, Plot buttons and a checked AutoPlot checkbox)
- intensity file:** syn_result.eva (with Browse, BrowseN, Edit buttons)
- info file:** syn_info.eva (with Browse, BrowseN, Edit buttons)
- number of bins:** 5000
- minimum [A, 1/A, deg]:** 0
- maximum [A, 1/A, deg]:** 10
- increase to next bin[%]:** (empty)
- dead-spot [deg]:** (empty)
- probability weight:** yes
- exclusive counts:** no
- scattering axis of the sample:** none
- time of flight:** yes
- correct tof to distance:** no
- flight path [cm]:** (empty)
- sample-detector distance [cm]:** 0
- time offset [ms]:** 0
- reference wavelength [Å]:** (empty)
- time interval begin [ms]:** -1.e10
- time interval end [ms]:** 1.e10

Task 3: Sample environment

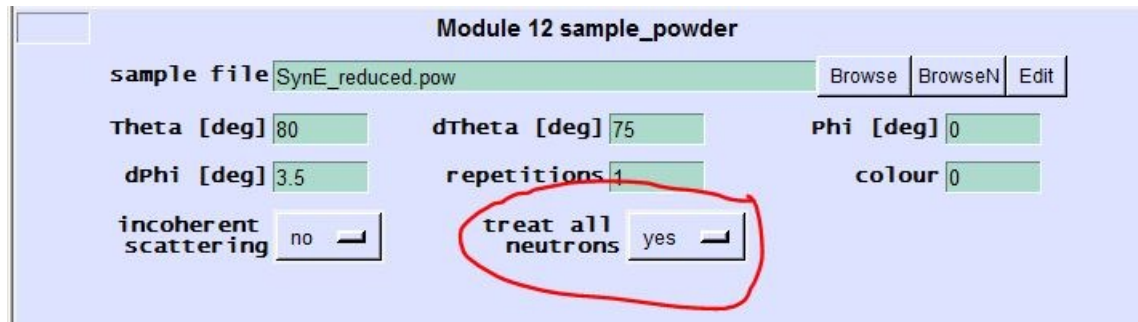
Add a sample environment (SE) to the instrument built in the previous task to study the effect of the background coming from scattering in the SE. Due to the modular structure of VITESS meaning that modules run independently of each other, two SE modules need to be included, one before (for incoming trajectories) and one after the sample (for trajectories to undergo scattering in the SE after diffraction in the sample). Trajectories coming from the SE can be marked with “color” and displayed separately by eval_elast.

Details:

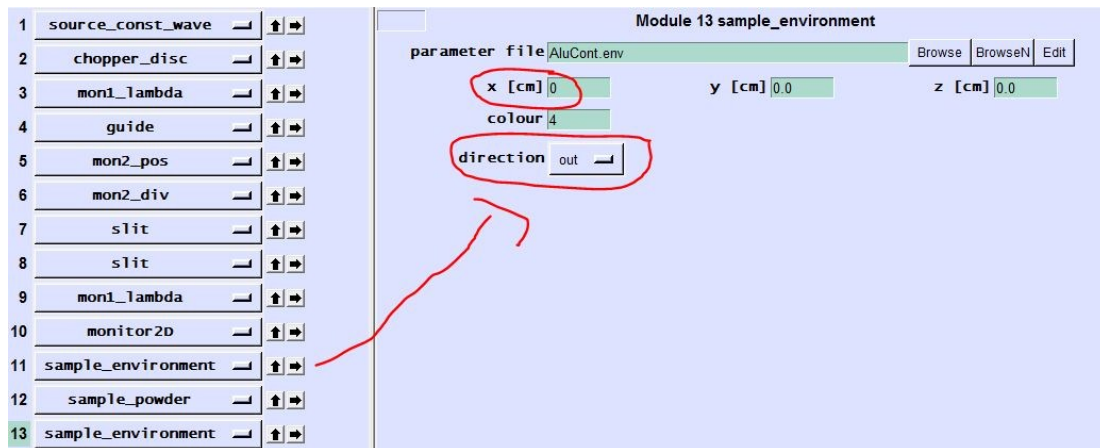
SE module before the (input files are provided):



Sample (input files are provided):



SE module after the sample (input files provided):



eval_elast: Create three eval_elast modules with different output file names and monitoring following color values: 0 for scattering from sample only, 4 for scattering from SE, -1 for all.

Task 4: Reflectometry sample

Create an instrument with a constant source, a chopper at 150 cm (as in tasks before), a collimation system consisting of 2 slits, a reflectometry sample, a detector and the eval_elast module. Reconstruct the (not normalized) reflectivity spectrum of a D2O sample. What happens if you switch on the incoherent scattering?

Details:

Source: Source size 2x4 cm², window 2x2 cm², **waveband 1 – 9 Å**, time 0 to 4 ms, use at least 2e8 trajectories.

Chopper: at 150 cm, parameters as before

Slits: Slit 1: 10 m away from the chopper, 1x2 cm²; Slit 2: 2 m away from slit 1; 0.25 * 2 cm

Sample: sample_reflectom module, input files provided

Module 12 sample_reflectom

parameter file: refl.ref [Browse] [BrowseN] [Edit]

reflectivity file: D2O.dat [Browse] [BrowseN]

mode: sample [v] axis of rotation: z [v]

reflection angle [deg]: 3

Offspecular scattering

offspecular scattering: Off [v]

Incoherent scattering

Incoherent scattering: On [v] ← First select „off“

Incoherent pathlength: 5.37

Detector distance: 150 Detector width: 40 Detector height: 40

Norm factor: 0.01

Detector:

Module 14 detector

General detector geometry

array (first or intermediated part)

geometry: flat [v] type: area/volume [v] usage: normal [v]

repetition: 1 detect color: -1 add color: -1

phi [deg]: 0 theta [deg]: 6 distance [cm]: 150

height [cm]: 50 width [cm]: 50 thickness [cm]: 1

number of rows: 200 number of columns: 200 number of layers: 1

hor. resolution [cm]: 0 vert. resolution [cm]: 0 resolution in x [cm]: 0

efficiency modifier: 0.9

lambda efficiency: [Browse] [BrowseN] [Edit]

absorber/convertor type: other [v]

gas pressure [bar] or solid layer thickness [cm]: 4 gas temperature [K] or atom density (solid) [10²⁷ 1/m³]: 293

Eval_elast:

Module 16 eval_elast

evaluation parameter

spectrum file AutoPlot

intensity file

info file

number of bins minimum [Å, 1/Å, deg] maximum [Å, 1/Å, deg]

increase to next bin[%] dead-spot [deg]

probability weight exclusive counts scattering axis of the sample

time of flight correct tof to distance

flight path [cm] sample-detector distance [cm] time offset [ms]

Monitors: Wavelength and time of flight vs wavelength after slit2; Horizontal divergence monitor after sample (check if the horizontal divergence = 6 °); 2D position after detector