Solutions to McStas hands-on exercise Reactor source diffractometer + TAS

by Linda Udby July 16, 2012

Source and monitors

3.

The unit of the intensity parameter I_1 is n/(s*cm^2*ster), where the cm^2 is the area of the source. The source is focusing at at an area dA=0.1m×0.1m monitor at r =1 m distance.

4.

Notice that all simulated neutron rays are monitored by the PSD and the full spectrum is respesented in the 0.1-10 Å range as shown in the left part of Figure 1. The intensity at the PSD is 1e14 n/s and it covers approximately $d\Omega = (0.1/1\text{rad})^2 = 0.01\text{ster}$, corresponding to a source intensity of $\frac{1e14\text{n/s}}{0.01\text{ster}} = 1e16$ n/(s*ster).

5.

The intensity on the PSD has decreased to 4e10 n/s since we are now tracing only part of the full spectrum, see the right part of Figure 1.

6.

The estimated solid angle of a dA=0.1m×0.1m monitor at r =1 m distance is 0.01 ster since Ω[ster] = dA/r^2. The source is emitting I_1=1e14 n/(s*cm^2*ster) but in a source area of 100 cm^2. Hence the total emitted intensity should be 1e14 n/(s*cm^2*ster)*100 cm^2= 1e16 n/(s*ster). Since the PSD covers 0.01 ster, the observed intensity should be 1e14 n/s if all the emitted rays hitting the detector are traced (i.e. if the focusing solid angle is as big or larger than the one spanned by the PSD). This is also what is observed in the top part of Figure 1. The intensity for the full spectrum is the same in a 100cm^2 size monitor whether the focus area is 100cm^2 as in the top part of Figure 1 or the focus area is 400 cm ^{2} as in the top part of Figure 2, but smaller if the focus area is smaller than the angle covered by the PSD as in the bottom part of Figure 2 since not all rays which could possibly hit the detector are traced.

If the number of traced neutron rays is increased, the number of rays traced to the monitors increase. The intensity on the monitors however does not change, the statistics simply improve ('Err' decreases).

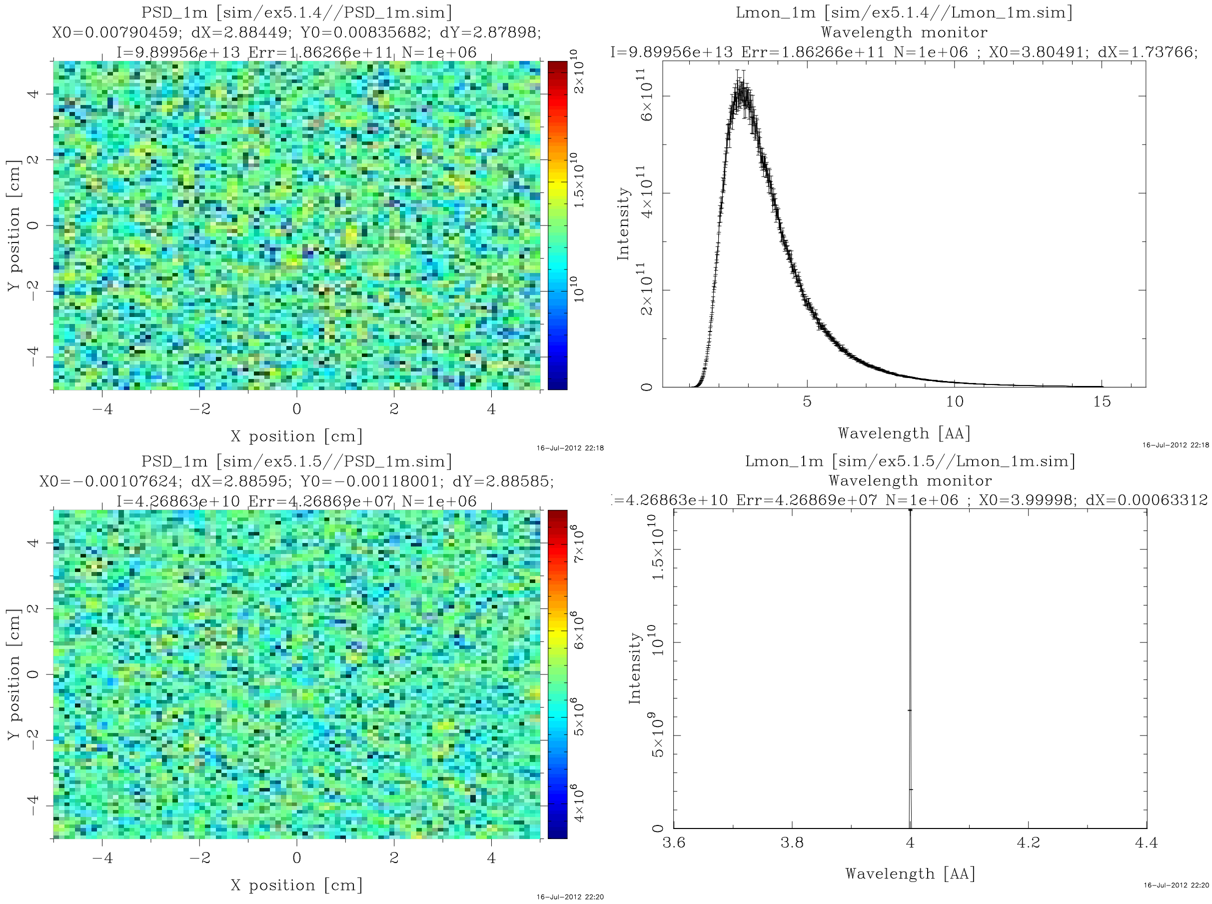

Figure 1: Beamprofile and wavelength distribution at 1m from the 100 cm^2 source with a focus area of 100 cm^2. In the top part of the figure the full wavelength spectrum is traced, in the bottom only $\lambda = 4 \pm 0.001$Å is traced.

Monochromator

3.

For $\lambda =$4Å neutrons, $k_i = \frac{2*pi}{\lambda} = 1.5708$Å^{-1}, which gives a scattering angle off the monochromator of

$$2\theta_M = 2 * \sin^{-1} \frac{\kappa_{\mathrm{PG(200)}}}{2 * k_i} = 73.21^\circ$$

5.

For Bragg scattering the monochromator itself must be rotated by $\Omega_M = 2\theta_M/2$. The intensity at the sample position in a scan of teh rotation angle of the monochromator is shown in Figure 3.

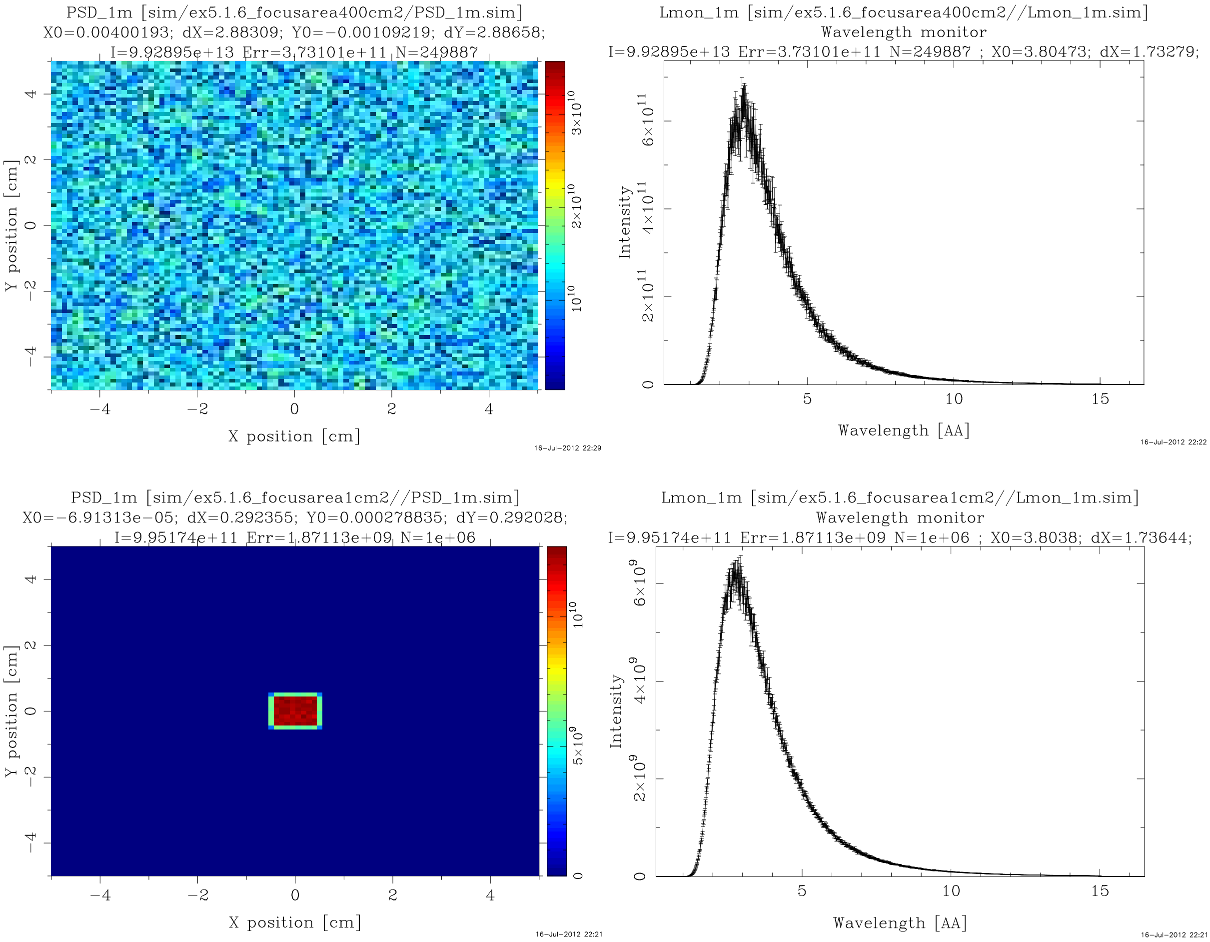

Figure 2: Beamprofile and wavelength distribution 1m from the 100 cm^2 source with a focus area of 400 cm^2 (top) and 1 cm^2 (bottom).

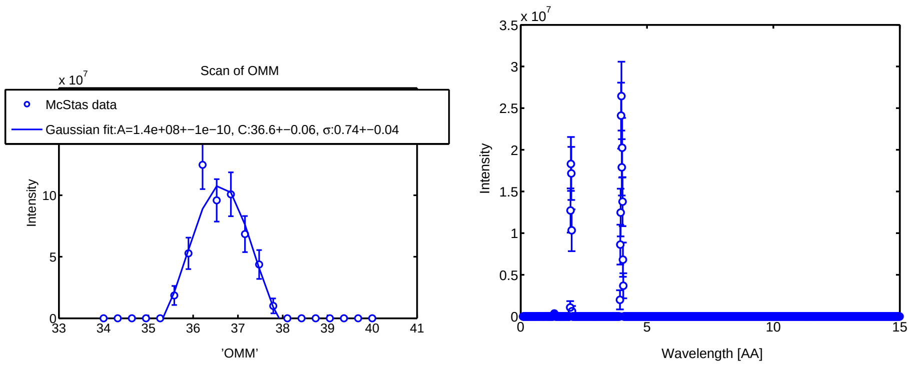

Figure 3: (Left) A scan of the monochromator rotation angle. The curve is a fit to a Gaussian.(Right) The neutron spectrum at OMM=36.6

6.

In order to get first, second etc order neutrons ($\lambda = 4, 4/2, \ldots 4/n$Å) scattered from the monochromator with scattering angle $\theta_M = 90°$ one would need to find a material with a scattering vector of

$$\kappa = 2k_i \cdot \sin(\theta) = 2.221\text{Å}^{-1}$$

From Figure 4 it is seen that a Bragg reflection is found at OMM=45 and that

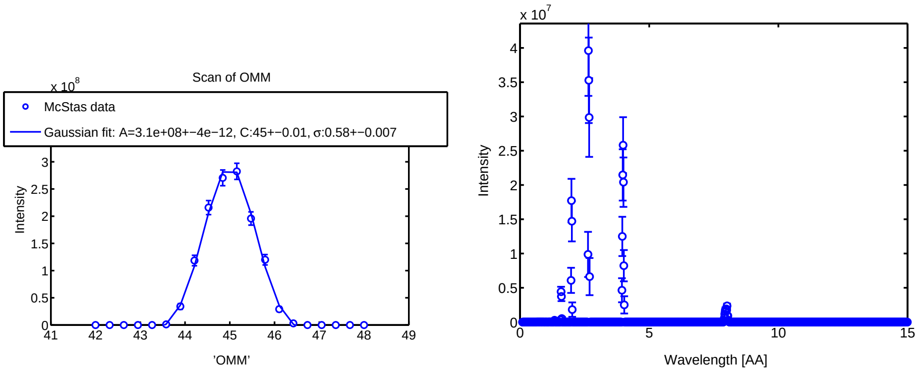

Figure 4: (Left) A scan of the monochromator rotation angle for $2\theta_M = 73.21°$. The curve is a fit to a Gaussian.(Right) The neutron spectrum at OMM=45.0

7.

When the scattering angle is set to reflect second order ($n = 2$) neutrons from the monochromator

$$2\theta = 2 \cdot \sin^{-1} \frac{\kappa\lambda}{4\pi n} = 41.41°$$

it is seen in Figure 5 that a Bragg reflection with wavelength 2Å is found at the sample position when turning the monochromator to $\Omega_M = \theta = 20.7$.

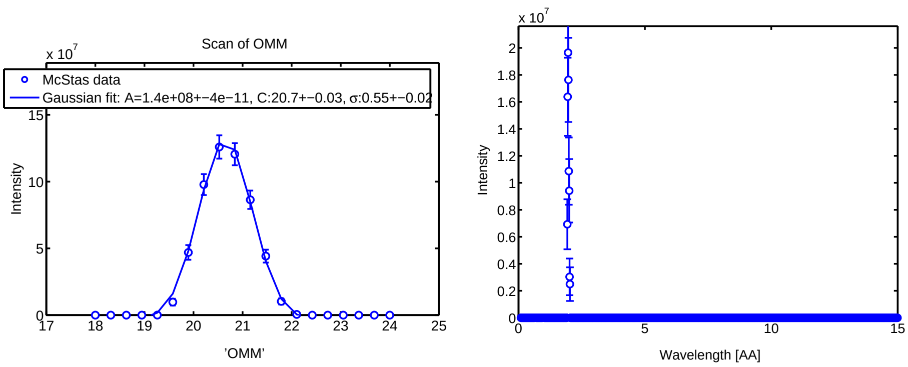

Figure 5: (Left) A scan of the monochromator rotation angle for $2\theta_M = 90°$. The curve is a fit to a Gaussian.(Right) The neutron spectrum at OMM=20.7

Vanadium Sample

The incoherent scattering from the Vanadium is seen in Figure 6

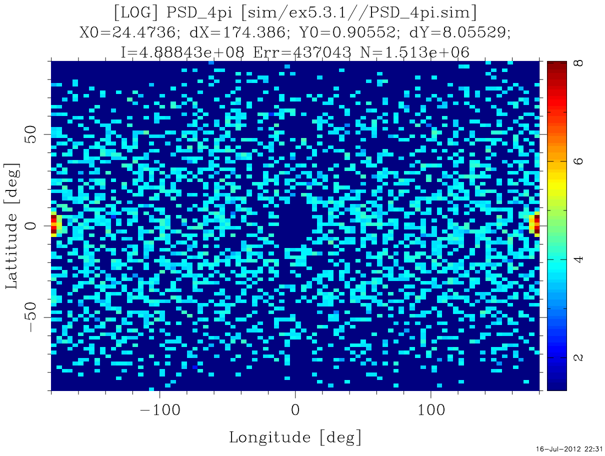

Figure 6: The scattering from the Vanadium sample

Powder Sample

The scattering on the detector from the 'powder sample' with two reflections is shown in Figure 7.

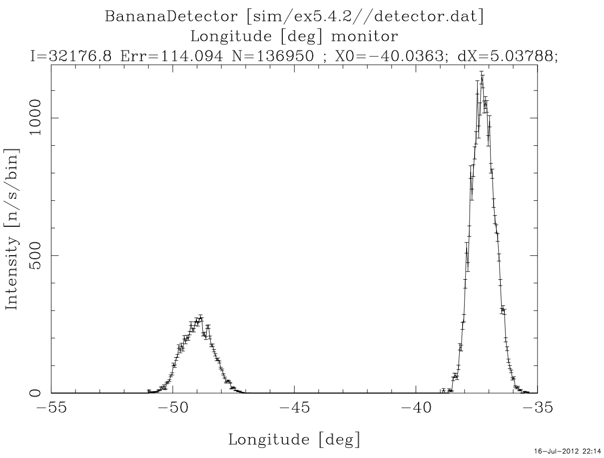

Figure 7: The scattering pattern from the Powder sample with two reflections

The scattering from the realistic powder sample is shown in Figure 10. It is seen that the q-resolution is best when scattering to the negative side $(2\theta < 0)$

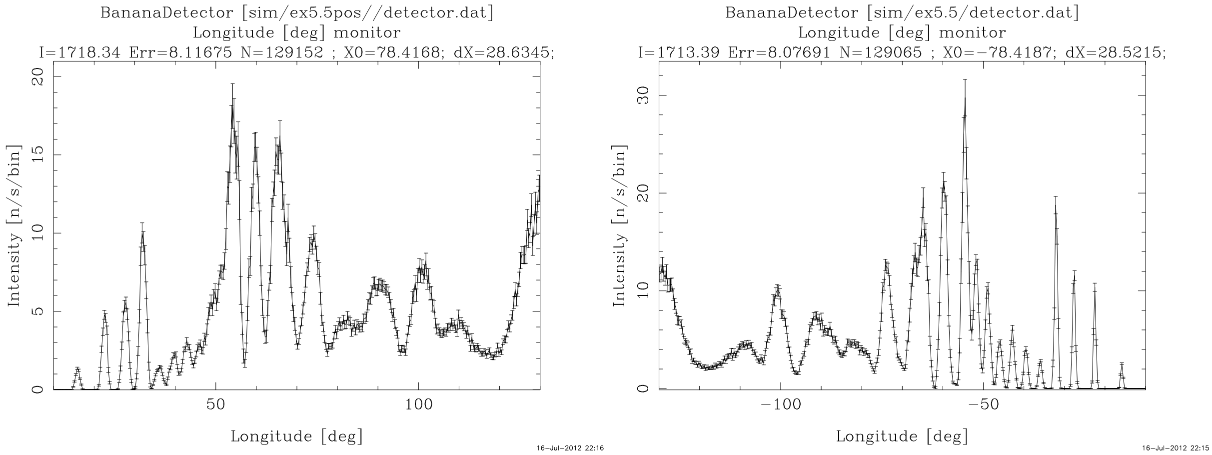

Figure 8: The scattering pattern of 2Å neutrons from the realistic powder sample. The left picture is scattering to the left (positive TT), the right is scattering to teh right (negative TT).

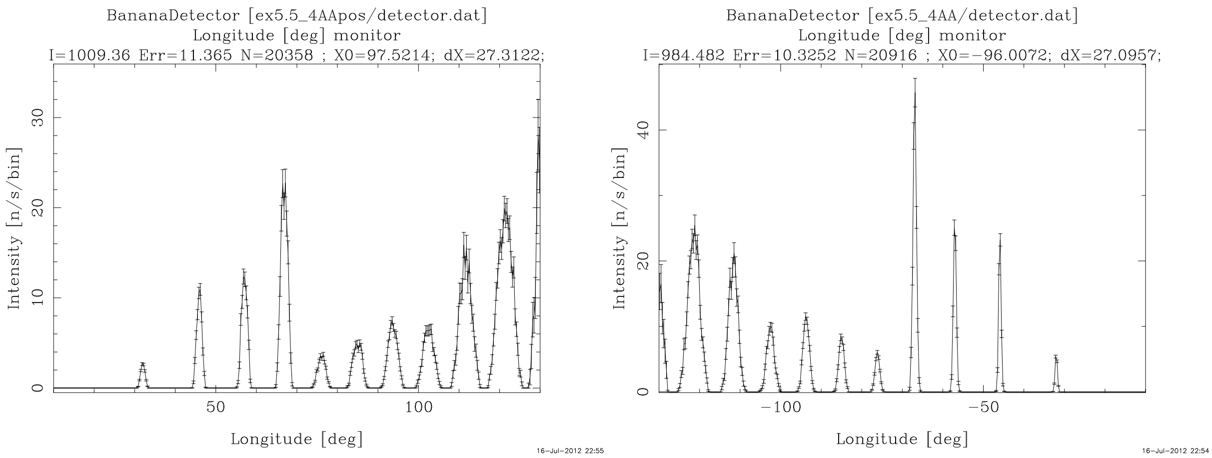

Figure 9: The scattering pattern of 4Å neutrons from the realistic powder sample. The left picture is scattering to the left (positive TT), the right is scattering to teh right (negative TT).

Analyser

An analyser crystal is inserted between the sample and detector and a single detector installed insted of the banana detector. The Bragg peaks from the sample are found by setting $2\theta_A = 2\theta_M$ and 2θ according to the position of some powderline of the pattern at the banana detector.
As observed at the banana detector the q-resolution is best when scattering to the negative side of the sample. The overall q-resolution of the instrument can be improved either by using colder neutrons (compare Figure 8 and 9) or horizontal collimation (not shown).

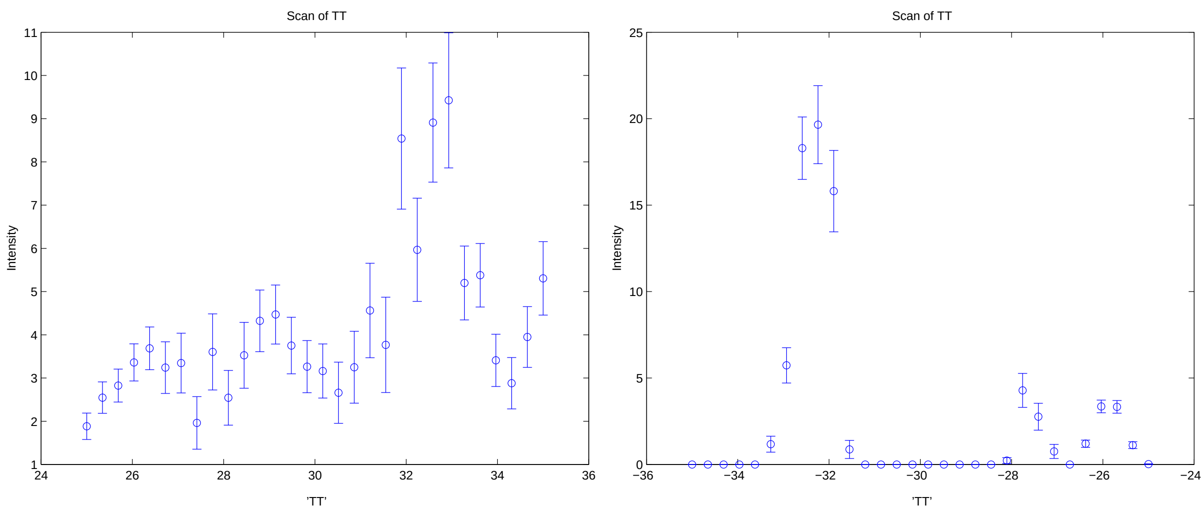

Figure 10: The scattering pattern from the realistic powder sample using a crystal analyser. The left picture is scattering to the left (positive TT), the right is scattering to the right (negative TT).