McStas tutorial 2005: DMC@PSI - A powder diffractometer

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DMC is a powder diffractometer situated at PSI, Switzerland. DMC is placed at the cold source and is optimized for high intensity and has a medium q-resolution.

In this assignment, you will use McStas to construct a model of DMC and perform a virtual powder diffraction experiment. You will compare results of your virtual experiment with actual data from the DMC instrument on the $Na_2Ca_3Al_2F_{14}$ substance.

If time allows, you are encouraged to suggest and investigate improvements to the spectrometer.

1 The cold source

The DMC cold source is made from liquid deuterium, D_2. The outgoing neutrons are not brought into complete thermal equilibrium with the cold source, so the energy/wavelength spectrum is not completely Maxwellian. However, it can be described as a sum of three Maxwellians. This is implemented in the source component `Source_Maxwell_3`. The correct parameters for this component are `width=0.085, height=0.16, T1=150.42, T2=38.74, T3=14.84, I1=3.67E11, I2=3.64E11, I3=0.95E11`.

Next to the source is an evacuated chamber, 1.50 m long. The chamber opening at the source is 0.08 m wide and 0.15 m tall; after 0.87 m, the chamber is 0.19 m wide and 0.19 m tall; and at the end of the chamber is it simply "tall and wide enough". You can safely assume that only neutrons traveling through this chamber will be worth simulating. The constricitons due to the chambers can be simulated by use of the component `Slit`.

1.1 Excercise

The chamber ends with an opening for the DMC take-out, 0.120 m high and 0.020 m wide. Simulate the neutron intensity in this opening (in neutrons/cm^2/sec). Record the energy and wavelength distributions to use for later comparisons. You can neglect neutrons with a wavelength below 1 Å (corresponding to an energy above 80 meV).

2 The guide system

Materials with positive scattering lengths have an index of refraction smaller than for vacuum. Like in optical cables, this allows for total reflection from a surface at low angles. This specular total reflection for neutrons will take place if the corresponding wave vector change is smaller than a certain material-dependent parameter. Above this value, the reflectivity falls off extremely fast.

A neutron guide can be made from Ni. This isotope has a large, positive scattering length, $b = 10.3$ fm, and the critical scattering vector is $\kappa_{Ni} = 0.0218\text{Å}^{-1}$.

Neutron guides may also be fabricated from multi-layers, where Ni (or ^{58}Ni) is the outermost layer. Here, total scattering is still seen up till κ_{Ni}, but the reflectivity remains high (50%-80%) until a higher value, $\kappa_{\text{crit}} = m\kappa_{Ni}$. The m-value is the main characteristic of a multi-layer guide. In the present DMC

guide, $m = 2$ is used. In the McStas component `Guide`, also the materials parameters α and W are used. The significance of these are described in the McStas component manual. We here simply assume the values `alpha = 4.38` and `W = 3e-3`.

The DMC beam system begins at the DMC take-out with a 30 m long guide system. You can assume the guide to be straight and with constant measures 0.120 m high and 0.020 m wide.

2.1 Excercise

Simulate the neutron beam profile (using a PSD), its intensity, energy distribution, and divergence at the exit of the guide. Compare this to the profile, intensity, energy distribution, and divergence at the same position if the guide was removed. Do you see any connection between the change in divergence and intensity?

3 Monochromator

Just after the guide exit (0.5 m downstream), the monochromator is placed. You can for a start assume it is a flat piece of PG crystal with a reflectivity of 80%. You will use the (002) reflection ($\tau = 1.87325$ Å^{-1}) to scatter the neutrons. The height of the monochromator is 0.12 m and the width is 0.20 m. Use the McStas component `monochromator_flat` with mosaicities of 30' both directions.

3.1 Excercise

You should select the "DMC standard" neutron wavelength of 2.4 Å. Calculate the scattering angle, 2θ and place a monitor at the sample position, 1.8 m from the monochromator centre. Assume that the sample is 3 cm high and 1 cm wide. Now, scan the monochromator orientation to obtain the maximum signal at the sample.

3.2 Excercise

Using the best setting found above, simulate the intensity, divergence and the energy distribution at the sample position. Do the same for the other "DMC standard" wavelength of 4.2 Å.

4 Collimator

4.1 Excercise

Insert a "Soller" collimator between monochromator and sample. Investigate collimations of 20', 40', and 60' and simulate intensity, divergence and energy distribution at the sample position. Compare to the situation without collimation. Select a collimation setting to use for the rest of the excercise.

5 Sample

5.1 Excercise

You are now ready to insert a sample. Use the component `PowderN` as documented in the component manual. Use the settings
`radius=0.005, h=0.03, pack=1, Vc=1076.98, reflections = "simple.dat", sigma_a=4*2.946, sigma_inc=4*3.418, frac=0.5, d_phi=5`
(`d_phi=5` limits the vertical angular range to $\pm 5^\circ$ to avoid wasting too many virtual neutrons).
Open the `simple.dat` data file and calculate the angle of the first reflection. Position a PSD monitor 1 m away from the sample at this angle and find the signal.

6 DMC multi-detector

The DMC detector has 400 channels with a 0.2° spacing, each 0.1 m tall. In other words, the angular spacing between detector 1 and 400 is 79.8° (total detector coverage becomes 80.0 degrees). This detector can rotate around the sample until the highest detector channel is at approx. 140°. In McStas, this detector can be inserted by means of `Monitor_nD` with input parameters (exactly)
`options = "banana, theta longitude bins=400 limits=[-39.9 39.9] auto y", xwidth = 2, yheight = 0.1, filename = "My_datafile"`

6.1 Excercise

Test the new detector set-up. Try to simulate incoherent background counts in all detector channels (by setting `frac=1` on the `Powder_N` you can suppress the powder lines). Try to vary the collimation of the incoming beam and see how this affects the signal.

7 A full virtual experiment

Exchange the `simple.dat` by the `na2ca3al2f14.dat` datafile. Investigate the best setting(s) for the multi-detector for this sample.

7.1 Excercise

Perform a full virtual experiment by running a long simulation of the counts in the multi-detector. Use a 20' collimator after the monochromator.

7.2 Excercise

Qualitatively compare your results with the real measurement data, provided in the `dat.xye` (columns: 2θ,I,$\sqrt{I}$) ascii datafile. Discuss discrepancies.

8 Optional: Improve your instrument

In this problem, you should optimize your instrument with respect to intensity and/or q-resolution. Anything goes as long as it works.

A few suggestions to start with: Guide parameters and geometry, monochromator parameters and geometry, distances, collimations, detector dimensions.

The DMC instrument will be upgraded over the next few years, and you may be able to find a suggestion for improvement that is better than the planned. Perhaps you can save PSI a few million Swiss Francs?