ESS Thermal Powder Diffractometer

We will here build a simple time-of-flight powder diffractometer. The basic philosophy is that a polychromatic beam is sent on to the sample and the diffracted neutrons are counted in time-of-flight detectors covering a large part of the solid angle. To interpret the data, one applies the basic time-of-flight equation

$$t = \alpha \lambda L, \tag{1}$$

where $\alpha = m_{\rm n}/h \approx 252.7\,\mu{\rm s/m/Å}$. One then assumes that all detected neutrons are scattered elastically, whence λ can be calculated. In turn, the scattering vector q can be found from 2θ, the scattering angle found from the detector position:

$$q = 2k_{\rm i}\sin(\theta) = \frac{4\pi}{\lambda}\sin(\theta). \tag{2}$$

1 The ESS moderator

ESS is a long-pulsed source, with the most important parameter being the pulse length, here called d, and the repetition frequency, $f = 1/T$. Make a simple instrument using the ESS thermal moderator `ESS_moderator_long.comp`, which emit neutrons directly into a time-of-flight detector, verb+, simulating a typical thermal wavelength range.

Use the standard parameters for a thermal source, listed in the component; otherwise default parameters. Simulate only one pulse (set parameter `twopulses` to 0), and use $d = 2.0$ ms, $f = 20$ Hz, and `size=0.02`.

1. Place one time-of-flight monitor `TOF_monitor.comp` directly at the moderator, one at 6 m distance, and one at 149.9 m distance (these monitors are physically realistic). The monitors should have the same size as the moderator, and the moderator should focus on the 149.9 m monitor. Perform the simulation. Adjust the timelimits to see the full pulse.

2. Next, place wavelength sensitive (but unphysical) TOF monitors, `TOF_lambda_monitor`, at these three positions and repeat the simulations. Notice how a given time channel (in the physical TOF monitors) contains a sharper wavelength information at the long distance.

3. Third, it is under consideration at ESS to chance the source parameters to $d = 2.86$ ms, $f = 14$ Hz. This should have the same time-integrated flux as the previous setting, given constant peak flux. Confirm that by calculations and simulations. (In fact, the ESS monitor is normalized to constant time-integrated flux.)

2 Frame overlap

Go back to the first settings of d and f and turn on a second pulse of the moderator. Notice that some time channels at the 149.9 m monitor has ambigious wavelength information. This is known as frame overlap. To avoid this, the wavelength band, $\Delta\lambda$, of the neutrons must be limited by the frame overlap conditions, i.e. neutrons from two following pulses (time T apart) must not mix. This gives rise to $T \geq \Delta t = \alpha\Delta\lambda L$, or

$$\Delta\lambda \leq \frac{T}{\alpha L}. \tag{3}$$

In reality, this is performed by frame overlap choppers at distances of 10-50 m from the moderator. In the simulations, you will merely limit the simulated band to the calculated value . Set the lower wavelength to 0.5 Å.

3 Powder sample

Let us go back to simulating just one pulse and postpone the simulation of the guide system. We place a 6 mm diameter sample at 150.0 m distance from the source. Initially, use `Powder1.comp` with a reflection of $q = 5$ Å^{-1}. For time-of-flight detector, we use a cylinder of 2 m radius and 20 cm height. Use the component `TOF_cylPSD_monitor.comp` and focus on the detector.

1. Perform the simulation and see how the scattered neutrons display a band in the (t, θ) plot. You may like to place a beamstop, e.g. 1 m after the sample to avoid the direct beam.

2. To perform quantitative analysis, place a 10 mm wide TOF detector at 90 degrees scattering angle, simulating a vertical stripe of pixels in the TOF detector (use `Arm` and place it after the perimeter of the cylidrical TOF monitor. Notice that the picture you reach resembles the moderator time structure (you may need to simulate up to 1E8 rays to see this). This information can be transferred into information on q.
   Calculate the percieved value of q and the peak width, dq.
   (Hints: think about the zero point in time and the total neutron flight path).

4 Resolution chopper

The resolution found in the experiment above is clearly too coarse, since you typically will need resolutions of $dd/d \approx 10^{-3}$ in the 90 degrees bank. To improve the resolution, we place a chopper at 6.0 m. It should have a radius of 0.35 m, an angular opening of 4 degrees, and spin with the source frequency (20 Hz).

1. Repeat the simulations and notice how both the time structure at 6 m and the time signal in the 90 degrees detector became significantly sharper.

2. Place a counter-rotating chopper just after the first one (negative `omega` and negative `t_0`). Notice how this again improves resolution. For even better resolution, one can spin double speed.

5 A realistic spectrometer

Now, this is only a simple mock-up of a real spectrometer. To perform the full simulation, a guide system is needed, and the moderator should have the full size of 12×12 cm^2 and focus on the guide opening. Although this sounds simple, there are a number of pitfalls, in particular the simulation time will increase dramatically. Therefore, this modification is not a part of this course, but could prove a good homework problem.