Experimental report

01/04/2016

Proposal: **1-10-24** **Council:** 10/2014

Title: Use of TOF analysis of pulsed, monochromatic neutrons to suppress incoherent scattering from 1H containing materials

Research area: Methods and instrumentation

This proposal is a new proposal

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Samples: $CaSO_4.2H_2O$
$(NH_4)H_2PO_4$

Instrument	Requested days	Allocated days	From	To
D7	8	6	07/05/2015	13/05/2015

Abstract:

Within the instrument development programme at the ESS, there is a new type of powder diffractometer that is based on pulsed, monochromatic beams, possible as a result of the high time-averaged brilliance of the ESS source. This opens up new experimental possibilities where the Time of flight (TOF) channel can be used to perform a range of energy dispersive measurements, such as simple multi-wavelength powder diffraction. However, it should also be possible to use the TOF channel to separate inelastic incoherent scattering from 1H containing materials and also provide some limited inelastic capabilities for the optimised powder diffractometer, through the use of a removable Fermi chopper on the secondary instrument upstream of the sample position. We have simulated this set-up in McStas and presented it to the Scientific and Technical Advisory Panel for diffraction at the ESS. They have requested experimental data to support the McStas simulation work and also investigate using polarised neutrons to provide enhanced information. The results from the experiment will be used to further optimise the instrument concept and update available McStas components.

Experiment report draft

The aim of the experiment was to explore the importance of background rejection using time of flight and polarization analysis simultaneously in an experiment where only the elastic information is of interest. D7 was first used in the standard diffraction mode to quickly get an overview of the powder spectrum for a range of temperatures, which is shown for a few temperatures in figure 1.

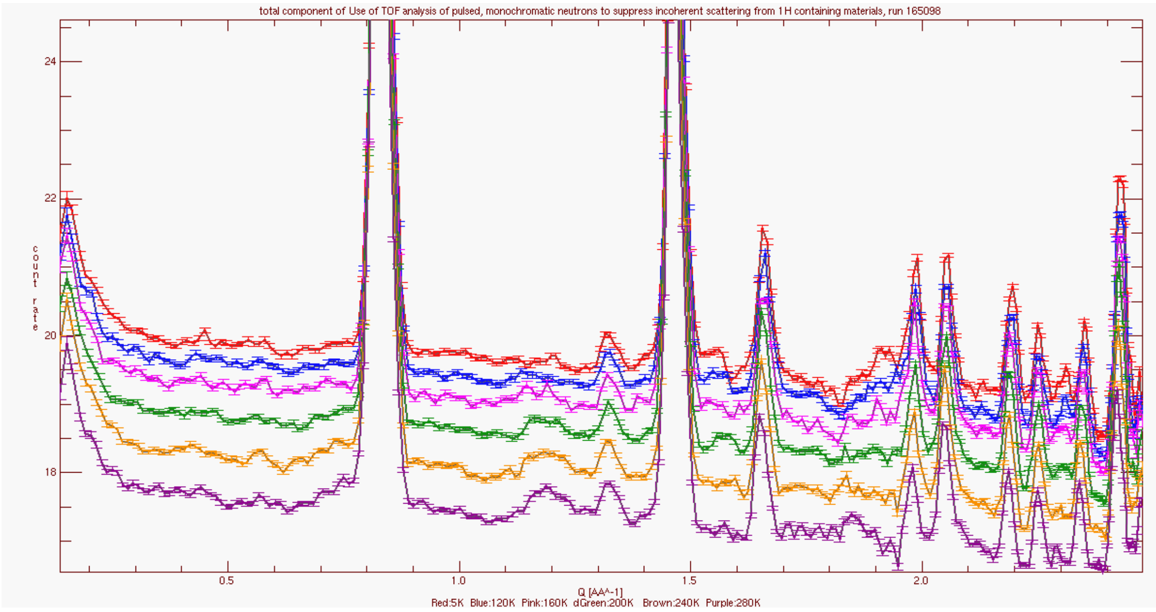

Figure 1: Diffraction data sets showing the total scattering at different temperatures. From the top intensity to the lowest, the temperatures are 5K, 120K, 160K, 200K, 240K and 280K. There have not been a background subtraction on these.

In figure 2 the separation of the total signal into the nuclear and spin incoherent is shown for the 280K measurement, which is done using the standard polarization analysis of D7. No background subtraction have been done for these measurements.

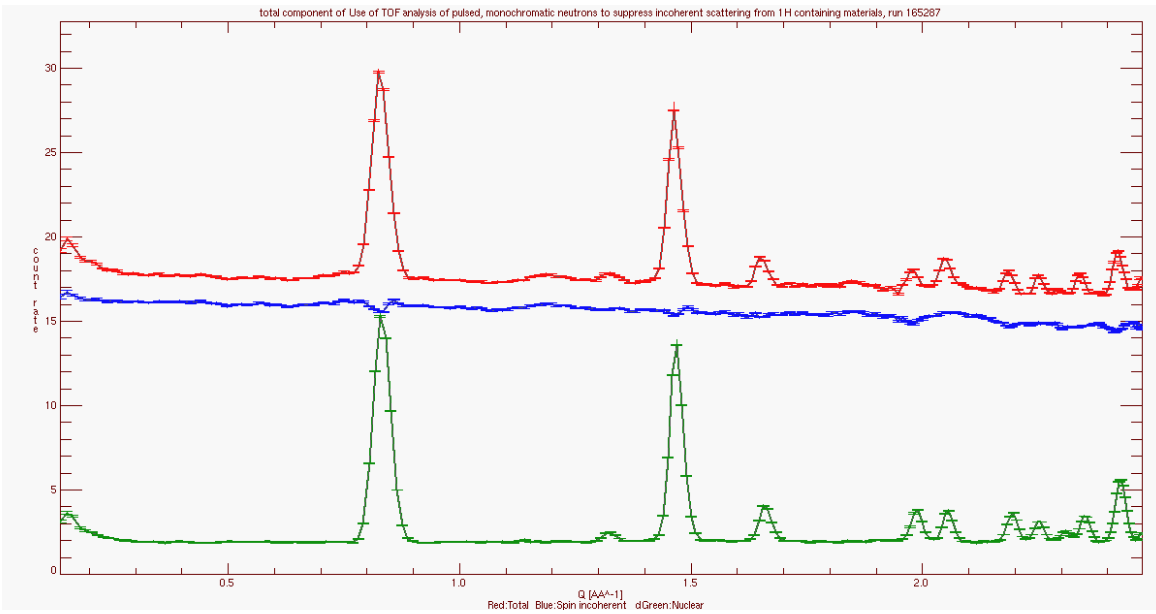

Figure 2: Diffraction measurement at 280K where polarization analysis was used to seperate the total scattering (red) into nuclear scattering (green) from the spin incoherent (blue).

By using the fermi chopper option on D7 we got the signal separated into time channels, which is shown in figure 3 for a range of temperatures. The inelastic signal is larger for higher temperatures as expected and a temperature of 280K was selected for a longer measurement with increased Q resolution.

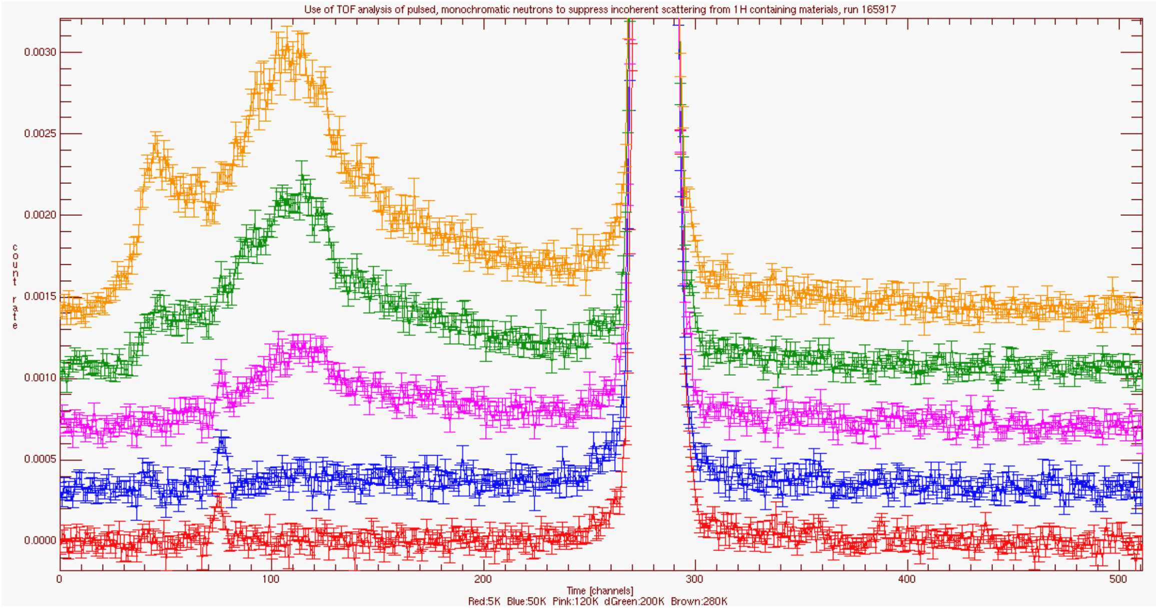

Figure 3: Time of flight measurement of the total scattering at different sample temperatures displaced for clarity. The temperatures are 5K (red), 50K (blue), 120K (purple), 200K (green) and 280K (orange). The elastic signal is at time channel 280, and the inelastic signal around time channel 100 is growing with temperature.

In figure 4 the time of flight signal for the longer measurement is split into spin incoherent and nuclear signal. We see most of the unwanted background is contained in the spin incoherent signal and would thus be possible to subtract without TOF analysis, but some remain in the nuclear channel.

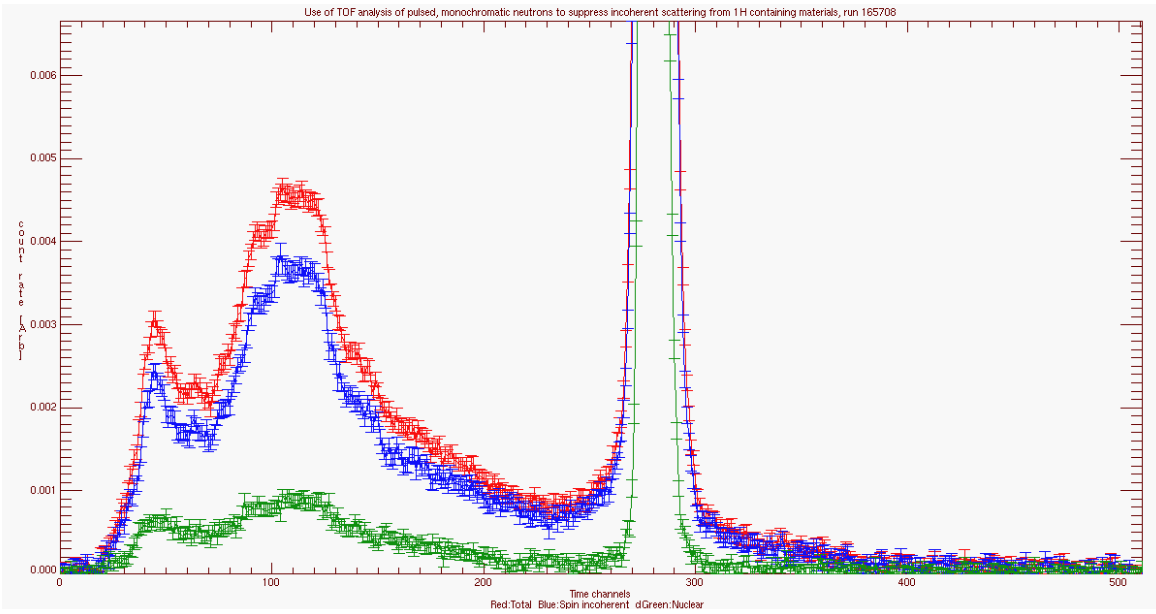

Figure 4: Components of the TOF signal separated using polarization analysis. The red curve is the total signal, while the blue is the spin incoherent and the green is the nuclear scattering. Elastic channel is around 280, while the inelastic signal is around 100.

On figure 5 the Bragg peaks of the material are extracted from the time of flight measurement using all time channels. As expected we see a high quality data set when the polarization analysis is used to extract the nuclear component. The quality of the spin incoherent part is much worse, and may be improved through more careful data analysis to take care of the difference in polarization detection efficiency for the different detectors.

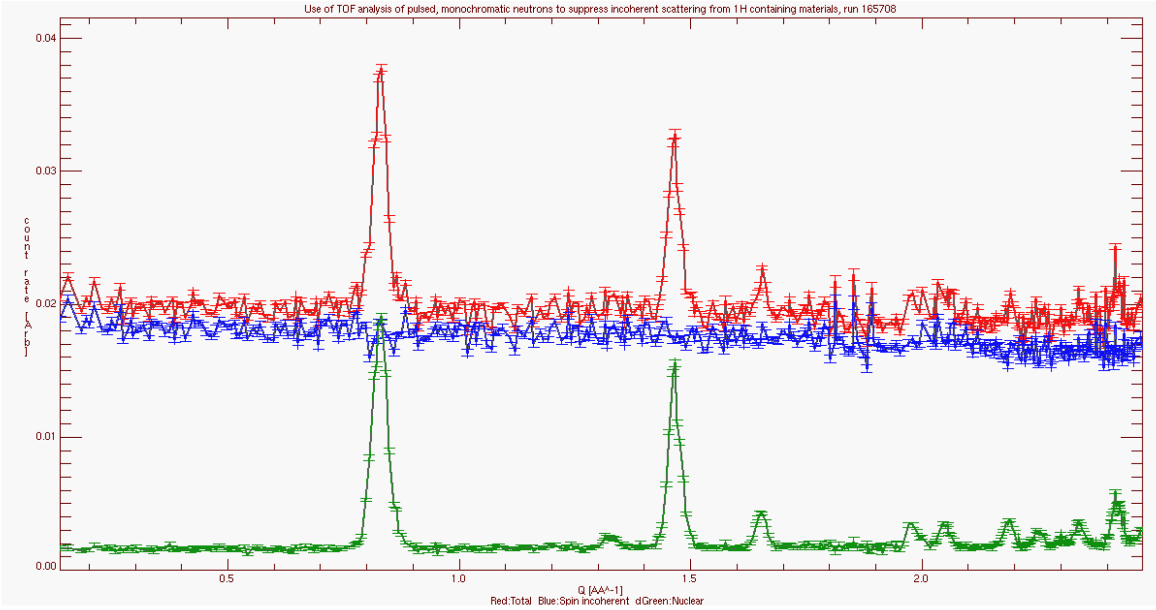

Figure 5: Polarization analysis used on the 280K TOF measurement, but summed over all time channels, and thus corresponding to a diffraction experiment. The total scattering in red, the spin incoherent in blue and nuclear in green.

The reason to use the time of flight option was to allow for selecting just the elastic part of the spectrum in order to remove the inelastic background. This is shown on figure 6, which is a zoom on a number of Bragg peaks at high Q where the inelastic signal is strongest (not shown). In this case it does not seem to be necessary to use time of flight analysis, as this reduces the incoming flux with a factor of 160 for a small increase in data quality.

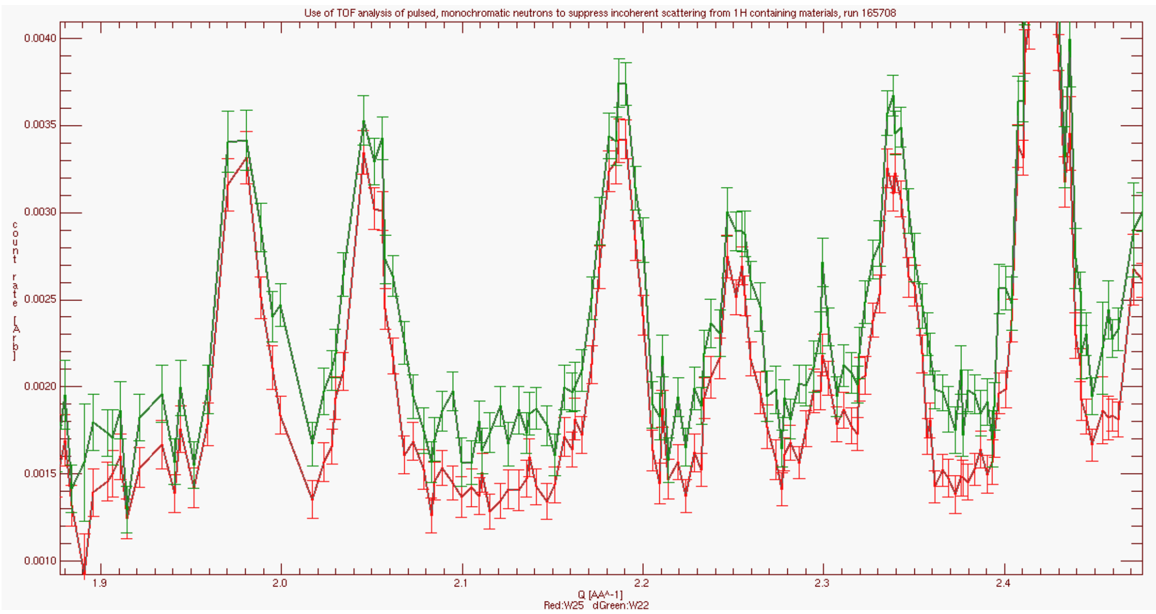

Figure 6: The nuclear signal from the time of flight polarization analysis, where only the data collected in the elastic time frame is used in the red data set, while the green data set with over all time channels.