Experimental Report

Proposal: **Council:** 10/2012 **TEST-2205** Title: XYZ polarization analysis accounting for the scattering altitude This proposal is a new proposal Researh Area: Main proposer: STEWART John Ross **Experimental Team:** STEWART John Ross WILDES Andrew **Local Contact: Samples:** Ho2Ti2O7 Req. Days All. Days Instrument From To D7 12/03/2013 14/03/2013 Abstract:

The nuclear contribution is linearly separable.

$$N = \frac{1}{6} \left(\frac{\partial \sigma^{x}}{\partial \Omega_{\uparrow}} + \frac{\partial \sigma^{y}}{\partial \Omega_{\uparrow}} + 2 \frac{\partial \sigma^{z}}{\partial \Omega_{\uparrow}} + \frac{\partial \sigma^{x+y}}{\partial \Omega_{\uparrow}} + \frac{\partial \sigma^{x-y}}{\partial \Omega_{\uparrow}} \right) - \frac{1}{12} \left(\frac{\partial \sigma^{x}}{\partial \Omega_{\downarrow}} + \frac{\partial \sigma^{y}}{\partial \Omega_{\downarrow}} + 2 \frac{\partial \sigma^{z}}{\partial \Omega_{\downarrow}} + \frac{\partial \sigma^{x+y}}{\partial \Omega_{\downarrow}} + \frac{\partial \sigma^{x-y}}{\partial \Omega_{\downarrow}} \right)$$

and finally the spin-incoherent scattering is given by

$$I = \frac{1}{4} \left(\frac{\partial \sigma^x}{\partial \Omega_{\perp}} + \frac{\partial \sigma^y}{\partial \Omega_{\perp}} + 2 \frac{\partial \sigma^z}{\partial \Omega_{\perp}} + \frac{\partial \sigma^{x+y}}{\partial \Omega_{\perp}} + \frac{\partial \sigma^{x-y}}{\partial \Omega_{\perp}} \right) - M$$

We have made extensive simulations of XYZ PA experiments on 2d detectors, and we believe we have arrived at a good scheme for separation of scattering contributions. In place of the normal 6-point measurement according to the XYZ scheme, we propose to measure the 10 cross-sections specified above.

We note from our calculations, however, that these equations will break down in the limit of significant quasi-elastic scattering, since such scattering will mean that there is a distribution of α and γ angles for each detector. (and indeed each detector pixel for 2d PSD detectors as on WISH for example)

In order to test the 10 pt scheme we have measured spin-ice $Ho_2Ti_2O_7$ and the diluted spin-ice $Y_{1.1}Ho_{0.9}Ti_2O_7$ on D7 using a wavelength of 4.8 Å.

Experimental Method

Using the D7 3d Hall probe, the X, Y, Z, (X+Y) and (X-Y) field directions were all set using the central adiabatic spin-turn coils. The field in each direction was set to be 10G. Quartz, vanadium and empty cell measurements were performed in each field direction. The spin-ice (HTO) sample was then measured at 300 K and 10 K for 40 mins in each polarization direction. From spin-echo measurements it is known that spin-ice is static at 10 K, but exhibits significant quasi-elastic scattering at 300 K. Lastly the diluted spin-ice sample (YHTO) was measured at 2 K, where previous spin-echo measurements have confirmed a static magnetic configuration.

The magnetic and the spin-incoherent cross-sections, as deduced using both the 6pt (XYZ) treatment and the proposed 10pt analysis are presented in figs 2 3 and 4 below for HTO at 300 K, HTO at 10 K and YHTO at 2 K respectively.

In each case we note that for the 6pt (XYZ) analysis, there is an upturn in the spin-incoherent cross-section and a concomitant downward dip of the magnetic cross-section in both samples at all temperatures. The low angle at which the (XYZ) equations break down is given by the point at which the spin-incoherent scattering starts to increase - and is approximately 30°. This roughly coincides with what was expected according to our simulations of D7.For the 300 K HTO data, we see that the 10pt analysis breaks down much more severely than the 6pt analysis. This again was expected from our simulations, and demonstrates that, although the 6pt method breaks down for out-of-plane scattering, it is remarkably robust with respect to inelasticity.

The low temperature runs of HTO at 10 K and YHTO at 2 K demonstrate that the 10pt analysis correctly separates the magnetic and spin-incoherent scattering - correcting for the out-of-plane effects suffered by the 6 pt analysis; *in the limit that the scattering is elastic.* This is clearly seen by the fact that the spin-incoherent scattering is flat at low scattering angles - as it should be. We hope to be able to quantify what allowable quasi-elastic linewidth is compatible with the 10pt method in the near future.

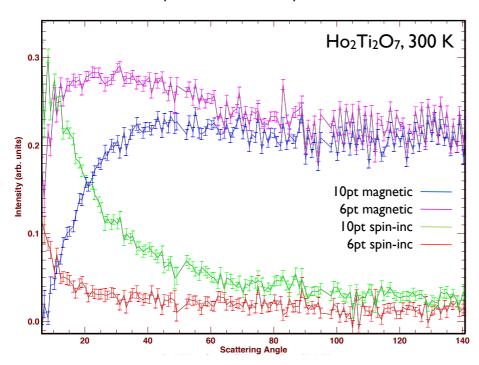


Fig 2. Magnetic and spin-incoherent cross-sections for HTO at 300 K. [red] 6pt spin-incoherent, [green] 10pt spin-incoherent, [purple] 6pt magnetic, [blue] 10pt magnetic

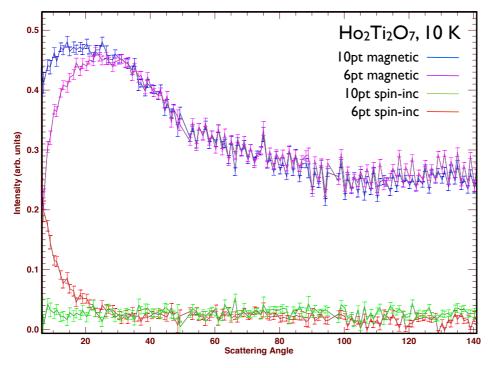


Fig 3. Magnetic and spin-incoherent cross-sections for HTO at 10 K. [red] 6pt spin-incoherent, [green] 10pt spin-incoherent, [purple] 6pt magnetic, [blue] 10pt magnetic

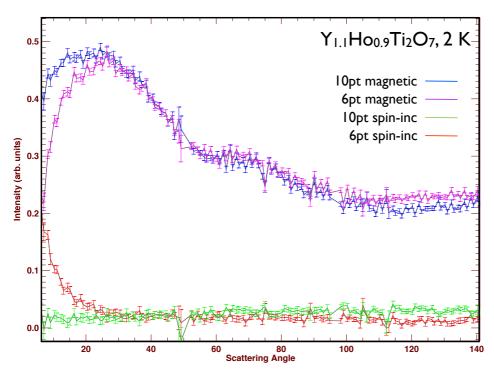


Fig 4. Magnetic and spin-incoherent cross-sections for YHTO at 2 K. [red] 6pt spin-incoherent, [green] 10pt spin-incoherent, [purple] 6pt magnetic, [blue] 10pt magnetic

The nuclear scattering is fully separable - linearly, and the 10pt and 6pt analyses of the nuclear scattering agree with one-another.

Conclusions

We conclude the following points:

- Out-of-plane scattering hampers the unambiguous separation of magnetic and spin-incoherent cross-sections on D7 below 30°
- For elastic scattering (and indeed for any isolated energy transfer, e.g. time-of-flight) the 10pt equations correctly separate the magnetic and spin-incoherent contributions
- When the scattering is quasi-elastic, the XYZ equations are robust, but the 10pt equations break down.
- In general, polarization analysis on a 2d multi-detector is possible **only for known energy transfers** i.e. either by measuring the time-of-flight or by ensuring that the scattering is "elastic"
- For general diffraction measurements of diffuse scattering and "total" scattering, the XYZ equations work well, above some low angle limit which depends on the vertical height of the detector array and vertical divergence of the beam.

Given that there is a measurable systematic breakdown of the XYZ equations below 30° on D7 we recommend that the 10pt scheme should be adopted as a standard measuring scheme on D7 in cases where the scattering is known to be elastic.