Experimental Report

Proposal: **5-42-272** **Council:** 4/2011

Title: Characterization of the magnetic correlations in Gd3Ga5O12

This proposal is a new proposal

Researh Area: Physics

Main proposer: **DEEN PASCALE Petronella**

Experimental Team: HOLM Sonja
JACOBSEN Henrik
DEEN PASCALE Petronella

Local Contact: FERNANDEZ DIAZ Maria Theresa

Samples: Gd3ga5o12
Gd3ga5o12

Instrument	Req. Days	All. Days	From	To
D9	7	12	12/12/2011	19/12/2011
			04/12/2012	09/12/2012

Abstract:

Gd3Ga5O12 is a geometrically frustrated compound and is one of the few compounds that does not order down to the lowest temperatures measured, 25 mK, despite antiferromagnetic dominant ex- change. Powder neutron diffraction revealed short range order, below 3 K, indicative of a spin glass or a cooperative paramagnet that nucleate around impurity centers below 140 mK leading to longer range contributions. Theoretical work suggested that the ground state is not caused by weak disorder but instead originates from the complex Hamiltonian in which competing small energy scales select the unusual ordering wavevector. In order to understand these small energy scales it is imperative to map a large area of S(Q). This proposal aims to do so using thin film single crystals on the hot neutron diffractometer D9, to minimise the absorption of the Gd isotope.

Experiment at D9 on single crystal $Gd_3Ga_5O_{12}$

Henrik Jacobsen
Nanoscience Center, Niels Bohr Institute, University of Copenhagen, DK-2100 Copenhagen Ø, Denmark and European Spallation Source, Tunavägen 24, Lund, Sweden

Pascale Deen
European Spallation Source, Tunavägen 24, Lund, Sweden

Maria Theresa Fernandez Diaz
ILL, Grenoble, France
(Dated: January 7, 2014)

We here report the results of the experiment performed at D9, ILL, in December 2012 on a single crystal of Gadolinium Gallium Garnet, experiment number 5-42-272. The experiment indicates that the RMC calculations based on powder diffraction on GGG give the correct picture of the magnetic order at low temperatures.

INTRODUCTION

The experiment began Monday 3/9 2012 at 9:00 and ended Sunday 9/12 2012 at 9:00. The aim of the experiment was to map out the short range magnetic order in a single crystal of GGG at low temperatures.

The wavelength chosen was $\lambda = 0.512$ Å, corresponding to $k = 12.2718$ Å^{-1}. We needed $\lambda < 0.8$ Å; othwerwise the huge absorption cross section of gadolinium would make the experiment impossible [1].

The sample was a $1 \times 1 \times 3$ mm single crystal of Gadolinium Gallium Garnet, $Gd_3Ga_5O_{12}$ (GGG). Before the experiment the orientation of the sample was determined with x-rays. The sample was mounted on the sample holder using a thin sheet of copper foil in such a way that ideally the (001) and (110) directions would be in the scattering plane. Due to high background, problems with the χ rotations and possible slight misalignment of the sample, we could not find the Bragg peaks for alignment. It was therefore decided to do the mapping anyway and figure out the exact orientation from the data afterwards. The following measurements were performed:

$\omega = \{-10, -9.8, -9.6, \ldots, 89.6, 89.8, 90\}$, $\nu = \{-2, 2\}$, $\Gamma = \{6, 9, 12\}$, where ω is the sample rotation in degrees, ν is the deviation angle of the detector with horizontal in degrees and Γ is the horizontal position of the center of the detector. With these 6 detector positions, a sufficiently large portion of the reciprocal space is mapped out, and the small step size in ω allows for precise determination of the position of Bragg peaks. Each of these measurements were done at 10 K (25 s/point, 22 hours in total), 0.175 K (20 s/point, 16 hours in total) and 0.05 K (25 s/point, 22 hours in total).

The sample had been at 10K for ~ 3 days before cooling to first 0.08 K and going to 0.175 K. The sample was left at 0.175 K for one hour before measurements started. After the measurements at 0.175 K the sample was cooled to 0.050 K and left at this temperature for one hour for thermalization before measurements started.

The minimum and maximum values of h, k and l in reciprocal lattice units (r.l.u.) were $h \in [-1.2, 6.8]$, $k \in [-1.2, 6.6]$, $l \in [-4.3, 5.5]$, corresponding to $|q| \in [0.98, 3.63]$Å^{-1}.

The relatively small q-values compared to k, combined with the 2d detector leads to detection of a significant amount of scattering away from the scattering plane.

DATA

The raw data have been converted to reciprocal lattice units in the following way: First of all, only part of the detector (circle with radius of 11 pixels at the center of the detector) has been used due to the circular slit in front of the detector. The peak positions as function of the sample rotation, ω and the scattering angle, 2θ were found. The (4 0 0) and (0 4 0) peaks were then used to calculate the orientation of the sample. The resulting alignment was then cross checked with a few other peaks.

Absorption corrections have not been performed yet.

Unfortunately, the $\Gamma = 6$ data are so close to the direct beam that a significant increase in background is observed here. We therefore omit the data from this detector position in the following.

An example of the data at 10 K is shown in Fig. 1. Here, a 0.4 r.l.u. wide cut was made around [h,k,0].

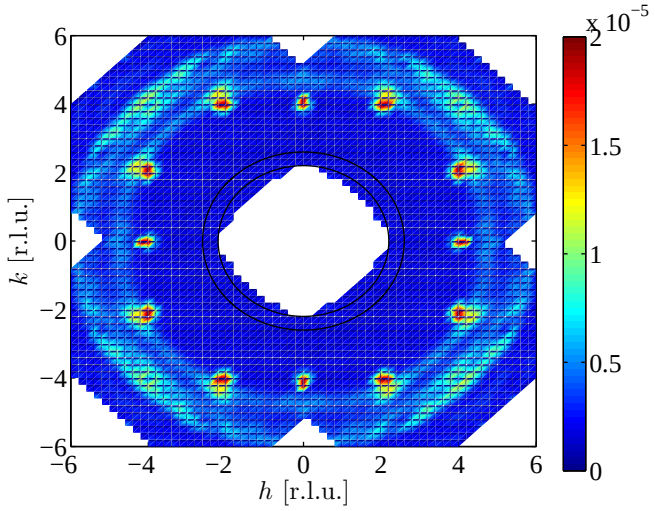

FIG. 1: A 0.4 r.l.u. wide cut around $(h, k, 0)$ of the 10 K data. Nuclear Bragg peaks are clearly visible. Also visible are the powder lines from Al and Cu.

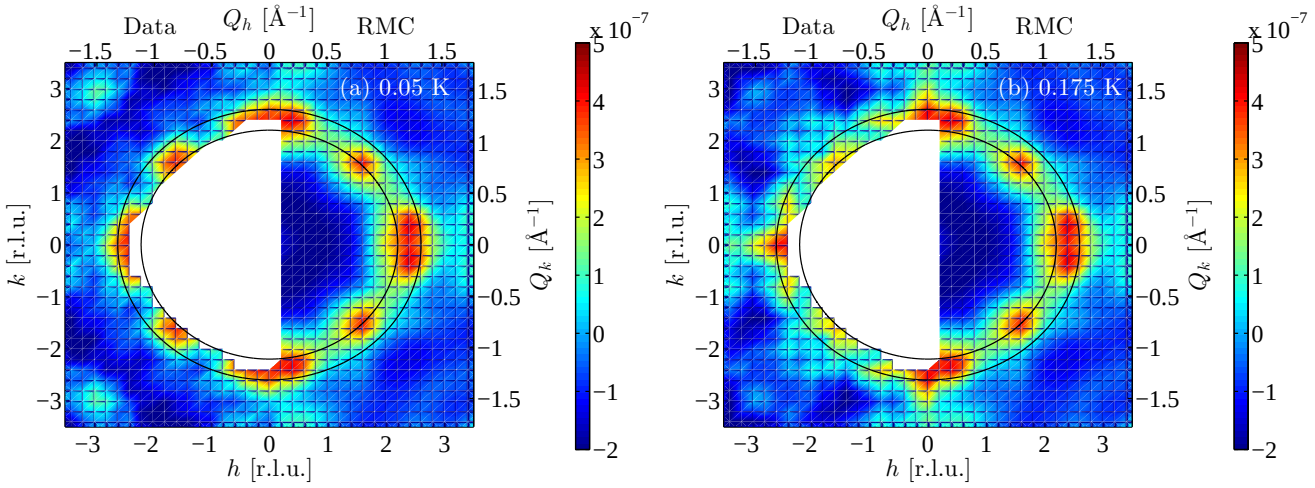

FIG. 2: The magnetic signal measured in this experiment by subtracting the 10 K data from (a) the 0.05 K data (b) the 0.175 K data. Left side of the figures show the data; the right side the RMC calculations. The black lines indicate the area in which a cut has been made and plotted in Fig. 3.

Data at 0.05 K and 0.175 K are shown in Fig. 2 and compared with Reverse Monte Carlo calculations (RMC) based on powder data from Petrenko et al. [3]. The RMC was performed using SPINVERT [2].

We now proceed to analyze the data in the $(h, k, 0)$ plane. A cut of thickness 0.4 r.l.u. around $l = 0$ was made in the experimental data which are shown in Fig. 2, here for 0.05 K. In this figure, also the RMC prediction of the magnetic structure at 0.175 K is shown. The scale of the data is counts/monitor, whereas the scale for the RMC calculations is arbitrary.

For a quantitative comparison of the data and RMC we cut the data as shown by the black lines in Fig. 2. This produces the plot shown in Fig. 3. Here we see quite nice agreement. The error bars are the statistical errors in the data.

CONCLUSION

In conclusion the experiment was succesful, yielding good quality data, even though the sample contained the highly absorbing ^{157}Gd isotope.

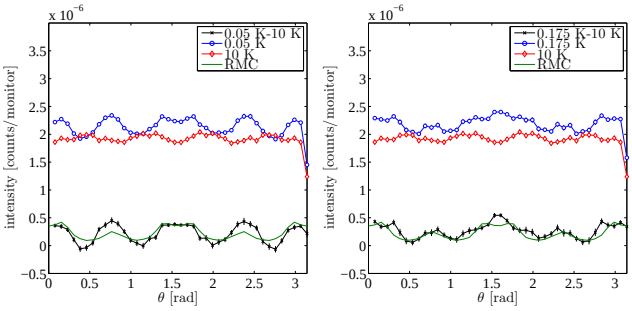

FIG. 3: A cut along the lines shown in Fig. 2. The RMC prediction has been scaled with the intensity in the data and displaced with the mean value of the data for better comparison. The error bars shown are the statistical errors in the data and are of the same size as the markers. (a) 0.05 K. (b) 0.175 K.

[1] G Leinweber, D P Barry, M J Trbovich, J A Burke, N J Drindak, H D Knox, and R V Ballad. Neutron Capture and Total Cross-Section Measurements and Resonance Parameters of Gadolinium. *Nuclear Science and Engineering*, 154:261–279, 2006.

[2] Joseph A M Paddison, J Ross Stewart, and Andrew L Goodwin. Spinvert: a Program for Refinement of Paramagnetic Diffuse Scattering Data. *Journal of physics. Condensed matter : an Institute of Physics journal*, 25(45):454220, November 2013.

[3] O.a Petrenko, D.McK Paul, C Ritter, T Zeiske, and M Yethiraj. Magnetic frustration and order in gadolinium gallium garnet. *Physica B: Condensed Matter*, 266(1-2):41–48, May 1999.