Experimental report

12/06/2017

Proposal: **5-31-2465**

Council: 4/2016

Title: Engineering magnetic competition in Mn3+xT1-xN

Research area: Physics

This proposal is a new proposal

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Samples: Mn3.6Sn0.4N
Mn3.5Sn0.5N
Mn3.2Sn0.8N
Mn3.5Ni0.5N

Instrument	Requested days	Allocated days	From	To
D20	3	3	07/07/2016	11/07/2016

Abstract:

Our theoretical studies of a range of antiperovskites, combined with magnetisation data, motivate a comparative study of the effect of temperature and field on the magnetic states of Mn3+xT1-xN (T=Sn, Ni). Our aim is to understand the mixed magnetism of Mn-containing metallic perovskites and to predict the existence of magnetic order-order phase transitions for applications such as solid-state cooling.

Engineering magnetic competition in $Mn_{3+x}T_{1-x}N$

The aim of the experiment was to determine the magnetic and nuclear structures of $Mn_{3+X}T_{1-x}N$ antiperovskites, with T = Ni and Sn and $x = 0$ and 0.5 for both, as a function of temperature in zero field and under a small applied field. The zero field measurements were to aid understanding of the magnetic sublattices as Mn is doped onto the T site. We aimed to measure under an applied field in order to determine its effect on the magnetic sublattices in the $x = 0.5$ samples, as we observe negative magnetisation in these due to the competing Mn sites.

Measurements were first performed on both T = Ni and Sn end-members, *i.e.* the $x = 0$ samples. Data were collected with neutrons of wavelength $\lambda = 1.54$ Å and a 90° take-off angle. Ceramic samples were loaded into 9 mm diameter vanadium cans. For Mn_3NiN data was collected between 10 and 300 K as $T_N = 260$ K continuously upon heating, whilst for Mn_3SnN temperatures between 10 and 550 K were measured upon continuous heating using the cryofurnace, as $T_N = 480$ K. For both samples the data collected was of excellent quality - see a representative diffraction pattern and Rietveld refinement for Mn_3NiN in Figure 1a. Refinement of the magnetic structure was possible across all temperatures for both samples.

For the $x \neq 0$ samples, sintered ceramic pellets, which were used to avoid crystallite reorientation in applied field, were loaded into 9 mm diameter vanadium cans. Data was collected using a cryomagnet under various different temperature and field treatments. Initially, samples were cooled to $T = 150$ K in zero field and data was then collected on warming in a small applied field ($H = 0.1$ T) to $T = 300$ K. Subsequently, the sample was cooled back to $T = 150$ K under the same applied field and measured on warming to 300 K. This final step was repeated again for fields $H = 0.5$ and 1 T. Unfortunately, analysis of the diffraction patterns measured with and without applied field shows that there is no significant difference between the two. Specifically, one would expect changes in the intensities of the magnetic Bragg peaks under appleid field, however example datasets collected on the $Mn_{3.5}Sn_{0.5}N$ sample in Figure 1b show this does not occur. Nonetheless, it is still possible to extract the magnetic structure as a function of temperature from Rietveld refinement of the data collected on the $x \neq 0$ samples and this analysis is ongoing.

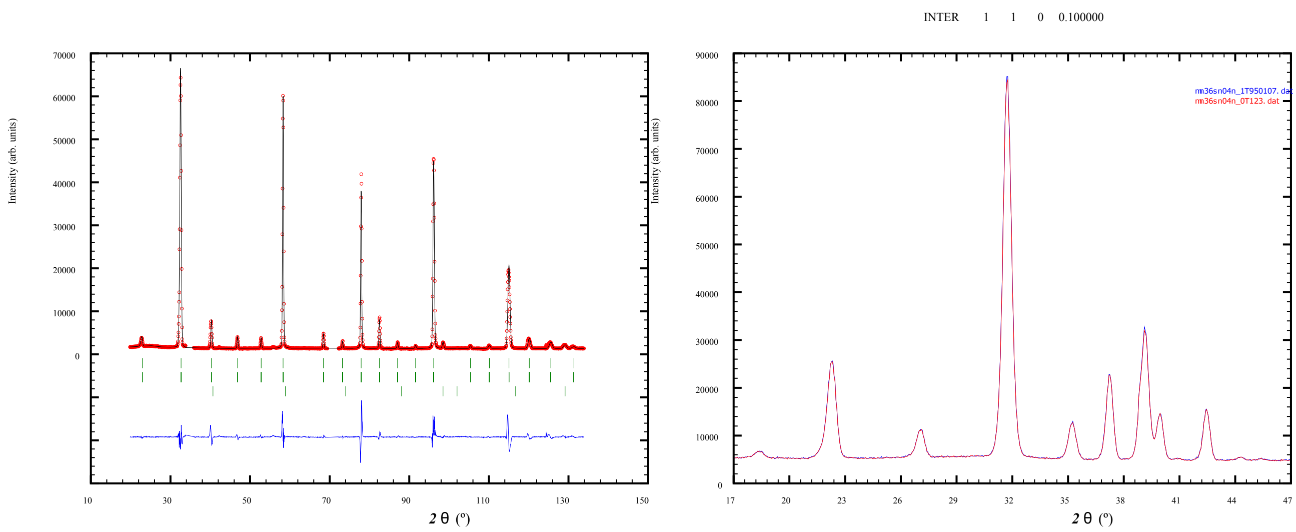

Figure 1: **a.** Typical Rietveld refinement of the neutron diffraction data collected on Mn_3NiN. **b.** Data collected on $Mn_{3.5}Sn_{0.5}N$ under 0 (red) and 1 T (blue) applied field.