Experimental report

14/05/2019

Proposal: **EASY-290** **Council:** 4/2017

Title: Magnetic structure of the ternary GdMn2Si2 compound and short-range magnetic order in Tb3Ni.

Research area: Materials

This proposal is a new proposal

Main proposer: **Andrei GUBKIN**

Experimental team:

Local contacts: Henry FISCHER

Samples: GdMn2Si2 / Tb3Ni

Instrument	Requested days	Allocated days	From	To
D4	24	24	08/06/2018	09/06/2018

Abstract:

RMn2Si2 (R is a rare-earth metal) compounds crystallize in a natural layered crystal structure and exhibit a rich variety of magnetic structures and magnetic phase transitions. This proposal is focused on the neutron powder diffraction study of magnetic structure of the GdMn2Si2 compound that contains highly absorbing Gd atoms. It is expected that one-off measurement at low temperature will be performed on the D4 instrument in order to solve the magnetic structure of GdMn2Si2.

We also plan to perform testing measurements on the Tb3Ni powder sample exhibiting a short-range magnetic order in a wide temperature range up to 5-6 times the Neel temperature. It is expected that the results of this experiment help us to prepare a normal access proposal for study of the short-range magnetic order effect in binary rare-earth intermetallic Tb3T (T=Co, Ni) and R5Pd2 compounds.

Magnetic structure of the ternary $GdMn_2Si_2$ compound and short-range magnetic order in Tb_3Ni.

ILL EASY-290 PROPOSAL
INSTRUMENT: D4
MAIN PROPOSER: A.F. Gubkin
LOCAL CONTACT: Henry Fischer

A series of neutron powder diffraction patterns for $GdMn_2Si_2$ sample were measured in the temperature range of 10K < T < 300K using D4 two axis diffractometer with a short neutron wavelength l=0.4959A. All the measured neutron diffraction patterns are shown as a function of temperature in the 2D plot (see Figure 1). It has been found that room temperature magnetic state with ordered Mn magnetic sublattice and disordered Gd magnetic sublattice can be described by the Shubnikov group *Pnnm*' which corresponds to the "AFmc" type [1] magnetic structure. Contrary, canted ferrimagnetic structure described by the Shubnikov group Pm'm'n was found to exist below T_{Gd}=54 K which was proved to be a magnetic ordering temperature for Gd sublattice.

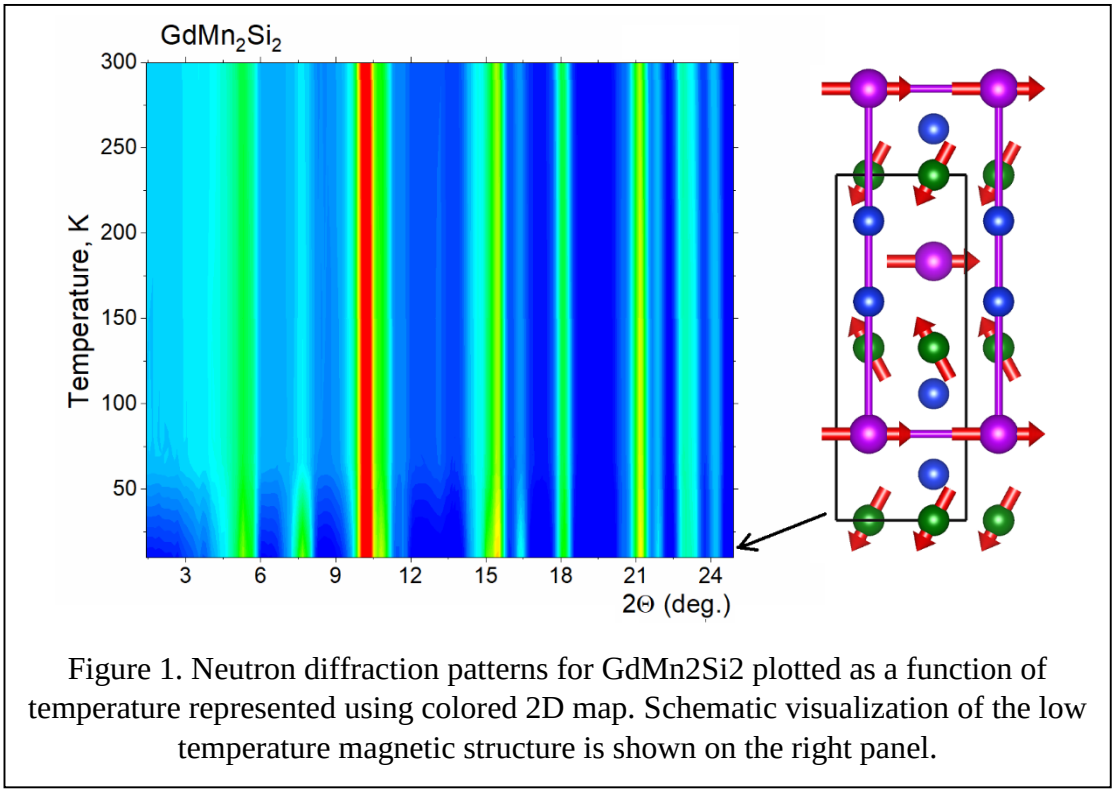

Figure 1. Neutron diffraction patterns for GdMn2Si2 plotted as a function of temperature represented using colored 2D map. Schematic visualization of the low temperature magnetic structure is shown on the right panel.

A series of neutron diffraction patterns for Tb_3Ni powder sample were measured in a temperature range of 10 – 300 K using D4 two axis diffractometer with a short neutron wavelength l=0.4959A. The short-range magnetic order was observed on the neutron powder diffraction patterns as broad diffuse maxima persisting in a wide temperature range below and above Néel temperature. An *ab initio* RMC refinement of the dynamical spin-correlations just above the Néel temperature at T = 65 K has been performed using SPINVERT program [2]. The spin-correlation function calculated from the spin configuration refined by SPINVERT in a 60Å-box (see Figure 2) reflects frustrated magnetic interactions in Tb_3Ni arising from the oscillating character of the RKKY exchange interactions. Correlations of the magnetic moments of the nearest-neighbor Tb atoms were found to be of the ferromagnetic type which is in agreement with the positive value of the paramagnetic Curie temperature obtained from the Curie-Weiss fit of the high temperature magnetic susceptibility. Contrary, negative correlations at the distances r ~ 6.8 Å and r ~ 9.5 Å,

which correspond to the *a* and *b* unit cell parameters, imply antiferromagnetic type interactions along the *a* and *b* crystallographic axes inherited from the long-range magnetic order.

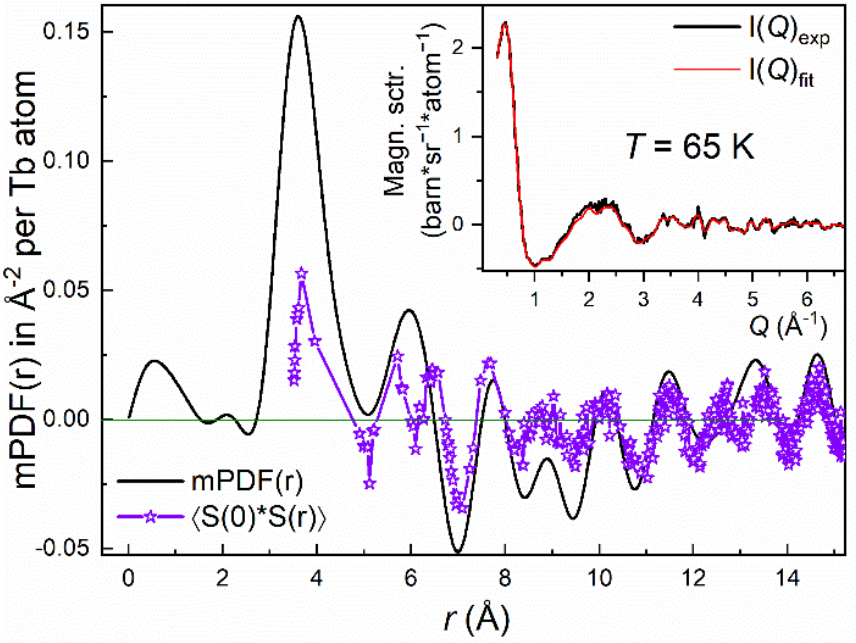

Figure 2. Magnetic Pair-Distribution Function obtained via Fourier transformation of the total magnetic scattering function measured from a powder sample of Tb_3Ni with the D4c neutron diffractometer (ILL, France) at T = 65 K (*shown in the inset*). The corresponding spin-spin correlation function revealing dynamical spin-spin correlations above the Néel temperature was calculated from the spin configuration refined by SPINVERT in a 60Å-box and laid on the mPDF function.

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References:

1. Venturini G, Welter R, Ressouche E and Malaman B 1995 J. Magn. Magn. Mater. 150197
2. J. A. M. Paddison, J. R. Stewart and A. L. Goodwin, J. Phys.: Condens. Matter 25 (2013), 454220.