Experimental report

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Proposal: 5-31-2602 **Council:** 4/2018

Title: Magnetic and crystal structures ofNiFe3O5

Research area: Materials

This proposal is a new proposal

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Samples: NiFe3O5

Instrument	Requested days	Allocated days	From	To
D20	2	2	01/10/2018	03/10/2018

Abstract:

Iron oxides have useful magnetic and electrical properties leading to extensive applications, e.g. the spinel ferrites. Using high temperatures and pressures we have synthesised the new phase NiFe3O5. We request 2 days on D20 with cryostat and furnace to collect high resolution diffraction patterns between 2 to 500 K from a 50 mg sample.We will determine the magnetic structure(s) of NiFe3O5 below the ~400 K magnetic ordering temperature and through the anomalies at 275 and 30 K in the susceptibility. We will also investigate possible structural changes associated with the magnetostriction and likely low temperature Fe2+/Fe3+ charge ordering, with associated Fe2+ orbital distortions, which is found in Mn and Fe analogues. The high flux and resolution of D20 are required in order to refine the magnetic moments at up to three cation sites for this complex material that is only available in small quantities.

$NiFe_3O_5$ neutron diffraction experiment

This experiment aimed to study the magnetic behaviour and the low temperature structure of $NiFe_3O_5$. Recent studies showed that members of the MFe_3O_5 family (with M^{2+} = Fe, Mn, Co and Ca) display fascinating electronic properties, such as electronic phase separation and multiple magnetic ground states upon cooling below 350 K. Polycrystalline sample of $NiFe_3O_5$ has been synthesised using high pressure and high temperature solid synthesis method. 50 mg of $NiFe_3O_5$ sample was used for powder neutron diffraction study. Diffraction patterns were collected at 1.5 K, 110 K, 220 K, 300 K and 400 K, using a helium cryostat at the D20 beamline. Rietveld fits to the obtained data revealed three magnetically ordered states when cooled below 300 K. Spin order of the octahedral sites of $NiFe_3O_5$ with a *k*-vector of [0 0 0] was observed at T_{N1} ~275 K, where the spins of the two sites are ordered antiferromagnetically along the *c* axis. An incommensurate magnetic transition was found below T_{N2} ~150 K. An additional magnetically ordered state, on top of the incommensurate magnetic structure, was observed when cooled below T_{N3} ~20 K. In the low temperature magnetic structure, the magnetic moments were found to propagate through the lattice with a *k*-vector = [½ ½ 0], doubling the *a* and *b* lattice parameters, with the spins of the three cation sites of $NiFe_3O_5$ ordered antiferromagnetically along *c*.

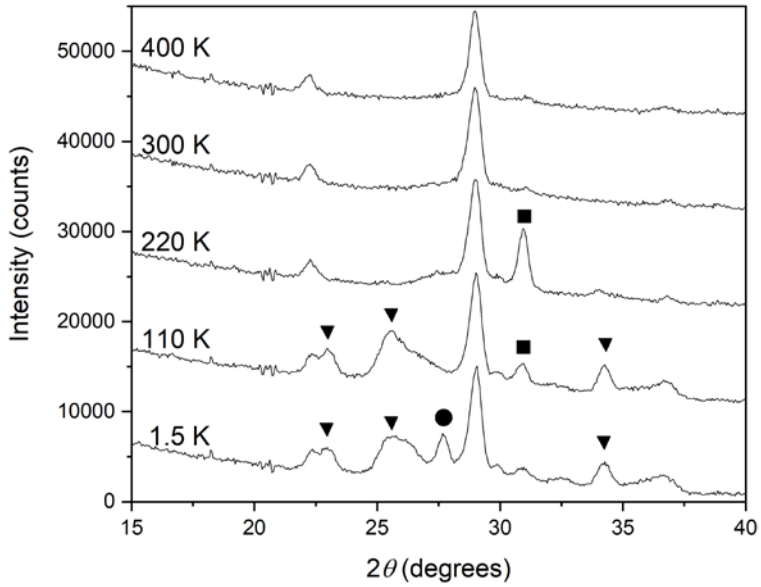

Figure 1. Temperature evolution of the neutron diffraction pattern of $NiFe_3O_5$. Magnetic peak contributions from magnetic structure with *k*-vector = [0 0 0], [0 0.38 0] and [½ ½ 0] are labelled by square, triangle and circle symbols, respectively.