Experimental report

27/01/2016

Proposal:	**4-01-1446**	**Council:**	10/2014
Title:	The magnetic density of states in NiPS3		
Research area:	Physics		

This proposal is a continuation of 4-01-1377

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Samples: NiPS3

Instrument	Requested days	Allocated days	From	To
IN4	5	5	27/07/2015	01/08/2015

Abstract:

NiPS3 belongs to a family of quasi-2D antiferromagnets on a honeycomb lattice. We have previously used neutron spectroscopy to establish that other members of the family are very good model magnets, namely: MnPS3, which is Heisenberg-like; and FePS3, which is Ising-like. NiPS3 shows novel effects in comparison, and we now wish to measure the magnetic density of states from a powder using time-of-flight spectroscopy. We have data from D7 showing a potential spin wave gap at 3 meV, but the measurement suffers badly for lack of flux and energy transfer band width. We now wish to measure on IN4 to establish the presence of the gap and to measure the full spin wave density of states. We would also like to search for a two magnon mode at 65 meV energy transfer.

The goal of this experiment was to measure the magnon density of states from a powdered sample of $NiPS_3$ on IN4. The MPS_3 compounds (M = Fe, Mn, Ni, Co) are quasi-two dimensional antiferromagnets where the transition metal atoms form a honeycomb lattice in the ab planes.

We have recently shown that, like MnPS3, its paramagnetic susceptibility is isotropic [1]. It has a magnetic structure similar to FePS3, withferromagnetic chains that are antiferromagnetically coupled. Previously published susceptibility data suggested that the susceptibility in the compound is anisotropic, and values for the anisotropy and J1 were derived from modeling the data with an anisotropic Hamiltonian with an added anisotropy. The magnitudes of the exchange and the anisotropy suggested that the spin waves would cover an energy bandwidth of ~15 – 20 meV, similar to $MnPS_3$ ($0.5 \leq \Delta E \leq 12$ meV) and $FePS_3$ ($15 \leq \Delta E \leq 40$ meV). Two magnon processes have also been reported in $NiPS_3$, measured using Raman spectroscopy. The excitations were found at $\Delta E \sim 65$ meV and are anomalously broad.

During a previous beamtime on the thermal time-of-flight spectrometer MARI at ISIS (see figure 1), we observed strong phonon modes at large Q, a feature around 1.2 $Å^{-1}$ and ΔE =3.5 meV which could be spurious and magnetic scattering at very low Q (close to the kinematic limits of the instrument) that appears around Q=0.6 $Å^{-1}$ and ΔE~6meV and disperses to Q=1.2 $Å^{-1}$ at ΔE~45 meV. We saw no evidence of magnetic scattering around ΔE =65 meV. The aim on IN4 was to obtain more information on the observed low Q scattering and to check the origin of the 1.2 $Å^{-1}$ feature.

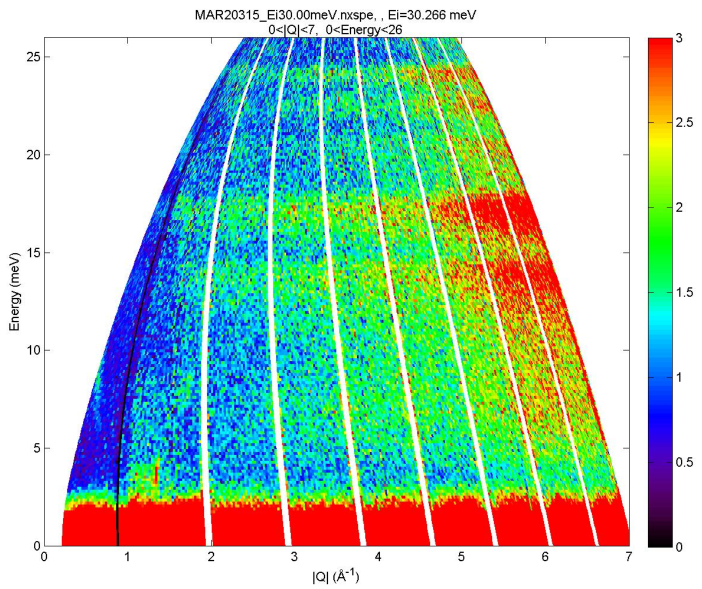

Figure 1 : MARI data at E_i=30 meV, 5K

Our 10.43 g powdered sample consisted of 3 pellets stacked inside an Al foil and held in a Cadmium holder which was inserted in a orange cryostat. The angle between the beam and the slab of cadmium was approximatly 45° The sample was cooled to base temperature (1.7K)

The main measurements were the following :
1) λ= 3.06 Å (E_i=8.74 meV). The results from this measurement(~15hrs) are shown in figure 2.

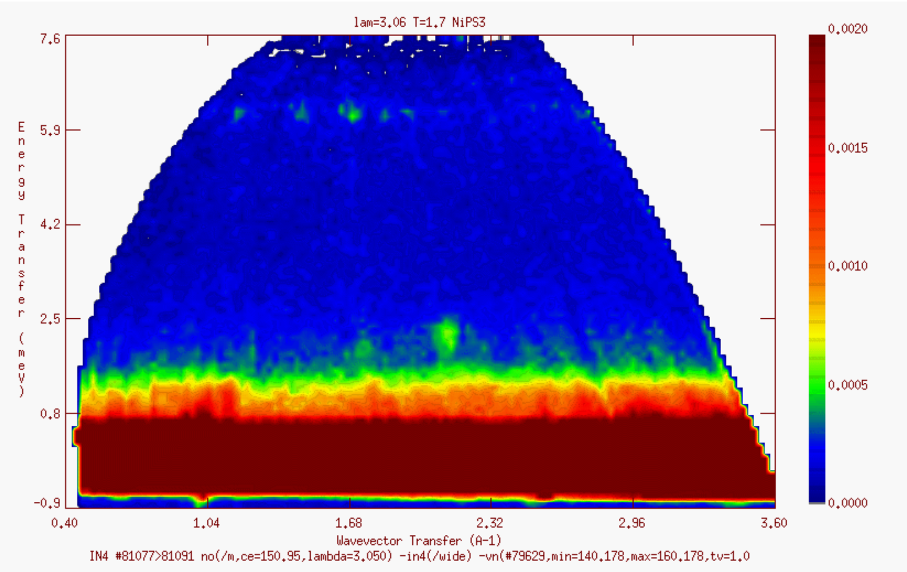

Figure 2 : λ =3.06 Å, 1.7 K, 15 hours

The feature around Q=1.2 $Å^{-1}$ and ΔE=3.5 meV observed on MARI in the previous beamtime is absent from these results. This confirms the spurious nature of the signal and it cannot be attribute to magnetic scattering. We conclude from this results that we do no oberve any magnetic scattering in the accessed (Q,w) space with λ =3.06 on IN4. Maps taken at additional temperatures (below and above Tn) and integrated over Q do not show any obvious magnetic scattering.

2) λ = 1.61 Å (E_i=31 meV,) The results from this measurement (~23hrs) are shown in figure 3.

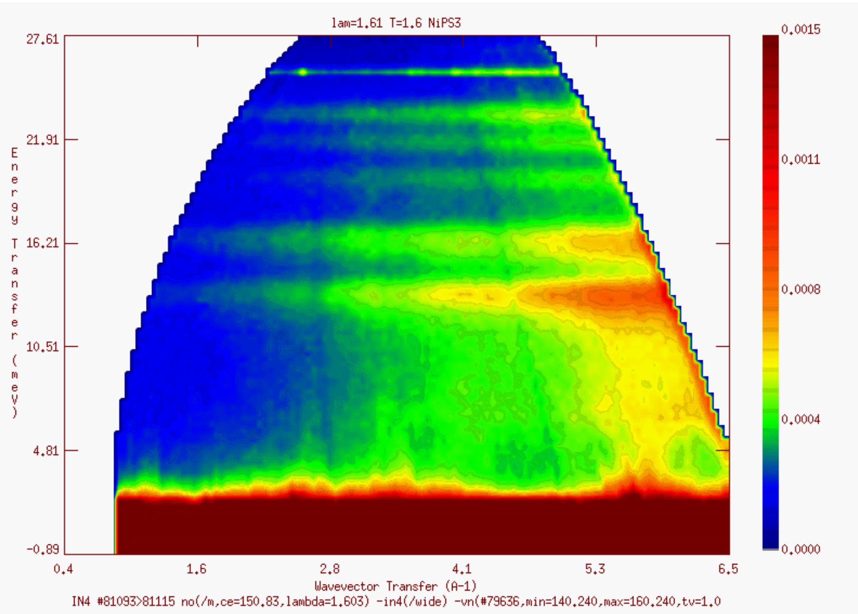

Figure 3 : λ =1.61 Å, 1.7 K, 23 hours

We observe the expected strong phonon modes seen on MARI. This map does not show any magnetic scattering. Due to the kinematic constraints of the instrument, we do not observe the low Q magnetic scattering seen on MARI.

From this experiment, we concude that the only evidence magnetic scattering in $NiPS_3$ is found at very low Q, with the mode appearing at Q=0.6 Å^{-1} and ΔE~6 meV. Due to the possible Q range accessed, we were not able to obtain more information on the low Q mode, but we plan to apply for a beamtime on BRISP, where lowest scattering angle is around 1°.

[1] A. R. Wildes et al., Phys. Rev. B 92 (2015) 224408