Experimental Report

Proposal: **INTER-296** **Council:** 10/2014

Title: Internal time on IN12

This proposal is a new proposal

Researh Area:

Main proposer: **SCHMALZL Karin**

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Samples: MnFe4Si3

Instrument	Req. Days	All. Days	From	To
IN12	6	6	28/04/2015	04/05/2015
IN3	0	1		

Abstract:

Background:

Compounds of the $Mn_{5-x}Fe_xSi_3$ system are magnetocaloric materials (MCM) where entropy changes of the magnetic material in a magnetic field is tied to adiabatic changes in temperature. The compounds in the Mn-Fe-Si system exhibit a moderate magnetocaloric effect (MCE). The environmentally friendly and cheap constituents make it a promising candidate for magnetic refrigeration. $MnFe_4Si_3$ (space group $P6_3/mcm$) is of particular interest as it has a T_C near room temperature.

So far studies in these systems have been mainly focused on the crystallographic and magnetic phase diagram in powder samples. In our group first single crystals have been grown and characterized concerning crystallographic and magnetic behavior.

The inelastic neutron scattering experiments on these compounds should shed light onto the relationship of the lattice and magnetic excitations and thus help to understand the fundamental mechanism of the MCE.

Aim of the experiment:

The aim of the experiment was to investigate the phonon and magnon dispersion at high (T=312K) and low (T=1.5K) temperatures. In particular the symmetry directions [001] and [100] are of interest and the results can be compared and interpreted with data from macroscopic measurements such as magnetization.

Experimental setup:

The instrument was set up in W-configuration. We used a double focusing PG monochromator and a PG analyzer. The data have been taken with a fixed $k_f=2.0Å^{-1}$. The single crystal (with a mass of about 7g) was mounted with the [100] – [001] directions in the scattering plane.

Results:

Inelastic neutron scattering measurements on IN12 (and complementary measurements on IN3) were performed on single crystal $MnFe_4Si_3$ at $1.5<T<5K$. Few scans were performed at high temperatures, i.e. 312K, but were not continued because of the high background that was observed (an about 8-10 times higher background than at 1.5K). In order to extract both, magnon and phonon branches, energy scans at constant q and q-scans at constant energies were performed. Scans were performed along directions [x 0 0] and [0 0 x]. Before fitting, every spectrum was analyzed carefully looking for spurions, in particular Al contamination, and the corresponding regions were cut out. Every peak (generated by magnetic or phonon excitation) was fitted with a Gaussian function.

Energy scans at constant q and q-scans at constant energies were mainly carried out at energies below 8meV looking for acoustic phonons (longitudinal and transverse) and magnon branches. Such scans were mostly conducted between intervals of +q and -q. Therefore every peak (if an excitation could be detected) was measured in focusing and defocusing mode. The exact position of a phonon (or a magnon) was evaluated by taking the average of focusing and defocusing value. In Figure 1 such typical scan is presented.

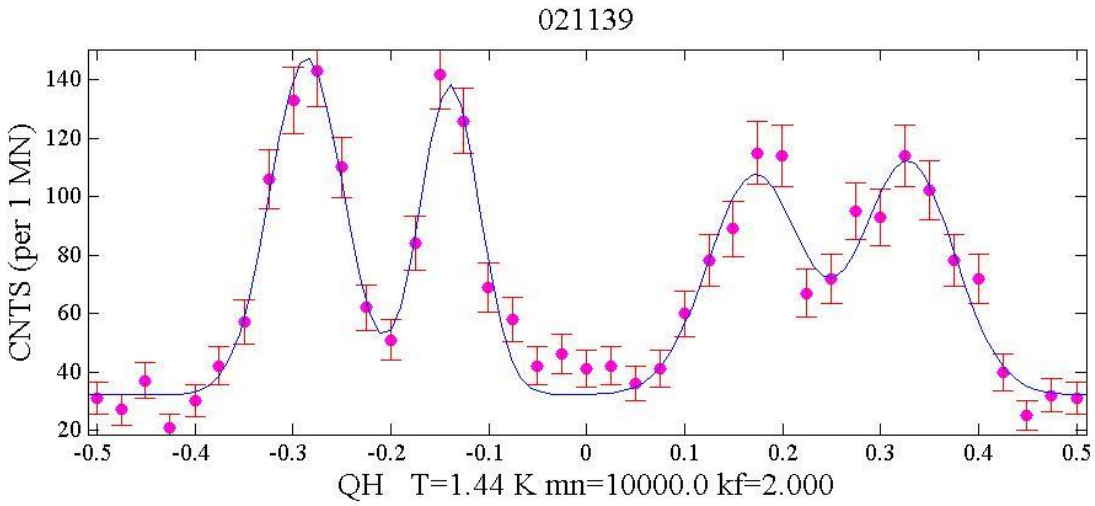

Figure 1: Transverse q scan (Qh, 0, 2) at 4meV on IN12 spectrometer.

Excitations were determined by combining collections of measurements performed close to the same Q-point (with the same zone center (1,0,0), (2,0,0), (0,0,1), (0,0,2)). Some preliminary results of the dispersion curves along a and c direction are shown in Figure 2. Peaks observed either in longitudinal or in transverse geometry can be attributed to lattice excitations, i.e. longitudinal acoustic (L.A., black in Fig. 2) and transverse acoustic (T.A., red in Fig. 2) phonons. It is expected from estimation of the magnetic form factor, that magnetic excitations generate peaks with significant intensities close to (2,0,0). The third branch (green in Fig. 2) is ascribed to possible magnetic excitations and has been measured in both longitudinal and transverse geometry.

In Fig. 2 the dashed lines are used as guides for the eyes. The points that appear in around 0.4 r.l.u. are still of unknown origin.

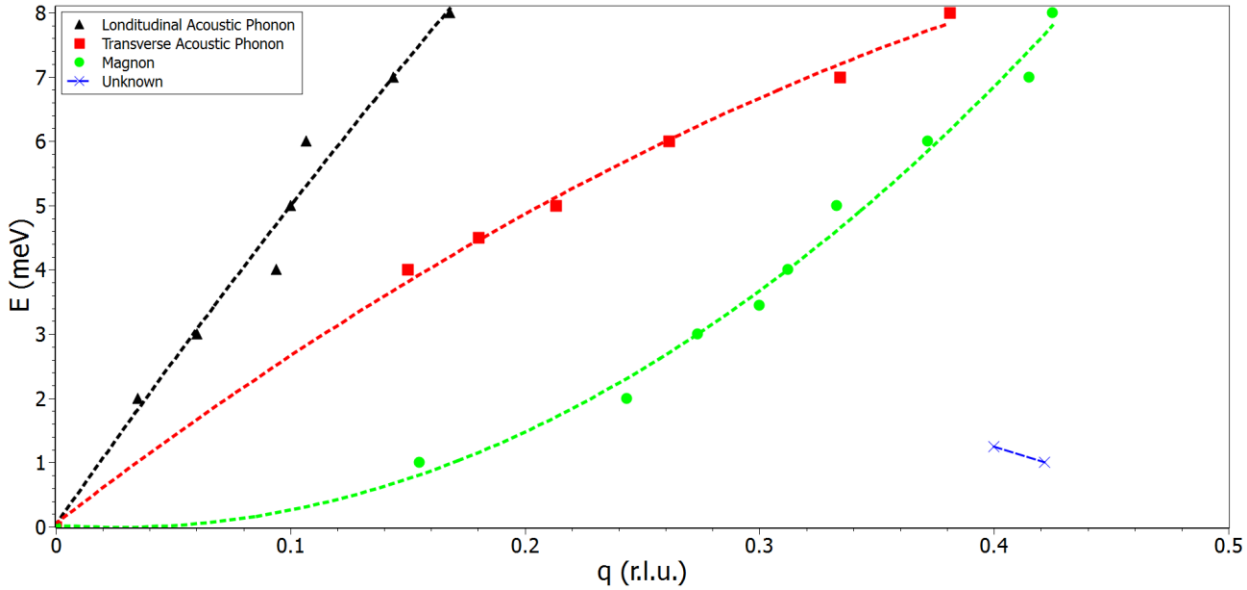

Figure 2: Preliminary phonon and magnon dispersion of $MnFe_4Si_3$ along a direction at T=1.5 K obtained on the IN12 and IN3 spectrometers.