Experimental report

29/10/2018

Proposal:	**4-01-1580**	**Council:**	4/2017
Title:	Effect of magnetic field on the magnetic excitation spectrum in the magnetocaloric compound Mn5Si3		
Research area:	Physics		

This proposal is a resubmission of 4-01-1542

Main proposer:	**Nikolaos BINISKOS**
Experimental team:	Nikolaos BINISKOS Mohammed AIT HADDOUCH
Local contacts:	Paul STEFFENS Stephane RAYMOND

Samples: Mn5Si3

Instrument	Requested days	Allocated days	From	To
IN12	7	0		
THALES	7	7	29/03/2018	05/04/2018

Abstract:

The aim of the proposal is to study the effect of an applied magnetic field on the magnetic excitation spectrum of the magnetocaloric compound Mn5Si3.

In a previous study performed at zero magnetic field, we evidenced a markedly distinct spin dynamics between the two antiferromagnetic phases AF1 (TN1=66K) and AF2 (TN2=99K) of Mn5Si3.

In particular, the higher temperature phase AF2 exhibits coexistence of diffuse spin fluctuations and well-defined spin-waves.

Since the AF1 and AF2 states are associated with direct and inverse magnetocaloric effect, respectively, the proposed experiment is crucial for revealing fundamental microscopic mechanisms associated with the magnetocaloric effect.

Background:

The search for more efficient use of energy has been leading to a growing interest for the research field of magnetocaloric materials. The magnetocaloric cooling process is based on the magnetocaloric effect (MCE). MCE is the reversible temperature change of a magnetic material upon the application or removal of a magnetic field. The MCE can be characterized as direct or inverse if a magnetocaloric compound heats up or cools down by applying an external magnetic field adiabatically. An entropy transfer between crystal lattice and the magnetic spin system has to take place. Among different compounds under investigation, the system $Mn_{5-x}Fe_xSi_3$ shows a modestly large MCE close to room temperature at low magnetic fields, which is promising for magnetic refrigeration applications. The parent compound Mn_5Si_3 on cooling undergoes a first phase transition at $T_{N2} \approx 100$ K toward a collinear antiferromagnetic ground state (AF2) and a second transition to a non-collinear antiferromagnetic phase (AF1) that occurs at $T_{N1} \approx 66$ K. Its specificity is to exhibit the inverse MCE in the vicinity of the AF1-AF2 transition.

Aim of the experiment:

The aim of this experiment was to investigate the in plane spin dynamics under field applied parallel to c axis in the AF1 phase, AF2 phase and in the PM state (the orthorhombic cell is derived from the ortho-hexagonal cell of the PM space group $P6_3/mcm$, therefore the a, b plane will be referred to as the ‘‘plane’’).

Experimental setup:

The ThALES spectrometer was set up in W configuration. A fully focusing setup was employed. We used a Si(111) monochromator, a monitor, slits before and after the sample and a PG(002) analyser. No collimators were used. Higher order contamination was removed using a Beryllium filter (Be) in the scattered neutron beam. All data have been collected with a fixed $k_f=1.5Å^{-1}$. The single crystal (with a mass of about 6g) was mounted with the [100] – [010] directions in the scattering plane inside a vertical 10T magnet.

Results:

Experiments were performed on a single crystal of about 1.5 cm^3 on the ThALES spectrometer. In order to investigate the spin dynamics under magnetic field along the [010] and [100] direction spectra were collected in three temperature regions: in the PM state (T=120K), in the collinear antiferromagnetic AF2 phase (T=80K) and in the non collinear antiferromagnetic AF1 phase (T<65K). Most scans were performed for an energy transfer of E<3.0meV around (1 2 0) and (0 3 0) Bragg positions.

Figure 1 shows typical E-scans obtained around (0, 3, 0) at 10K at different magnetic fields. In the INS spectra shown in Fig.1 a parasitic signal appears at about 1.7meV. The intensity and peak position of this parasitic signal seem to be field independent. For evaluating the spectra the following steps were followed: (i) the intense elastic line at E=0meV was masked, (ii) a constant background was assumed for all different magnetic fields (bgr=88(9) arb. units), (iii) the lineshape of the spurius scattering was assumed to be Gaussian and its peak position, width and intensity were fixed (center=1.69(2) meV, HWHM=0.24(1) meV, amplitude=234(17) arb. units) and (iv) the inelastic magnetic signal was fitted with the quasi-Lorentzian function. The results of this analysis are shown in Figures 2

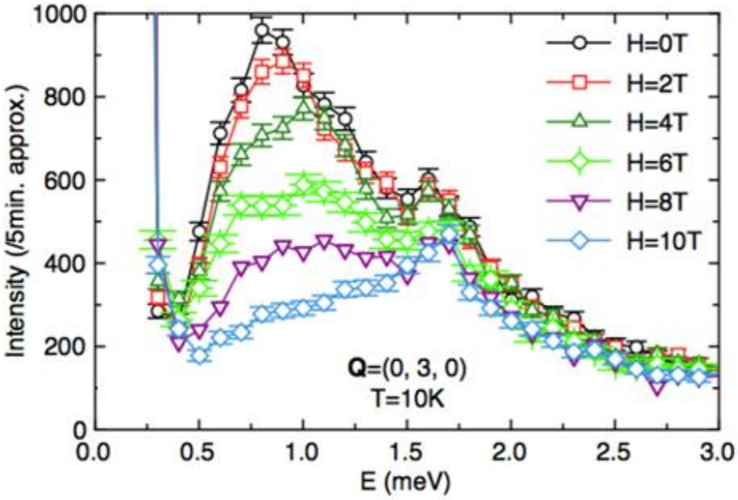

Figure 1: E-scan around (0, 3, 0) obtained at 10K at different magnetic fields. The lines are guides for the eyes.

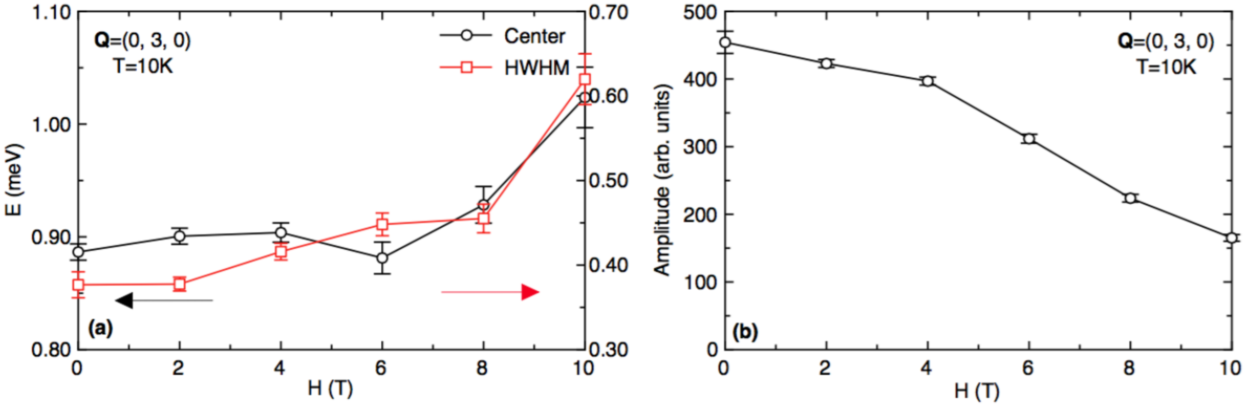

Figure 2: Fitting results for the inelastic spectra collected around Q=(0, 3, 0) at T=10K at different magnetic fields. (a) Magnetic field dependence of the spin gap and the HWHM. The corresponding values for the spin gap and the HWHM are given on the left and right vertical axis, respectively. (b) Magnetic field dependence of the amplitude. The lines are guides for the eyes.