Experimental report

23/03/2021

Proposal: 4-01-1682 **Council:** 4/2020

Title: Investigation of spin and lattice dynamics of the magnetocaloric compound Mn5Ge3

Research area: Physics

This proposal is a new proposal

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Samples: Mn5Ge3

Instrument	Requested days	Allocated days	From	To
IN8	7	0		
IN22	7	8	09/02/2021	17/02/2021

Abstract:

The study of phonons, magnons and their coupling is of great importance for the understanding of the mechanism of the magnetocaloric effect (MCE). Therefore, inelastic scattering measurements with a thermal triple axis spectrometer on the novel ferromagnetic compound Mn5Ge3 are highly important in order to highlighten the microscopic ingredients that favor a large MCE. Such a study was never performed before on Mn5Ge3. The results could provide new insights not only for magnetic refrigeration applications, but also for spintronic devices. The need to design functional materials connects with a fundamental understanding of magnetism and lattice dynamics.

Scientific background:
The intermetallic ferromagnetic Mn_5Ge_3 compound has attracted great scientific interest in the recent years because it is considered as a promising candidate material for spintronic and magnetocaloric applications. Mn_5Ge_3 exhibits a 2nd order phase transition from the paramagnetic state towards the ferromagnetic phase at approximately 295K. It crystallizes in the hexagonal space group $P6_3/mcm$, with two distinct crystallographic positions for manganese atoms (Wyckoff positions (WP) *6g* for Mn2 and *4d* for Mn1). The magnetic structure of Mn_5Ge_3 was determined by polarized single-crystal neutron diffraction, which revealed a different size of the magnetic moments on the *4d* ($1.96\mu_B$) and the *6g* site ($3.23\mu_B$). In both sites the magnetic moments lie parallel in the *c*-axis of the hexagonal unit cell. The magnetic entropy change, ΔS_m, is of 7.2 J/kgK for a magnetic field change of 5T near room temperature. In addition, electrical resistivity and magnetization measurements in Mn_5Ge_3 indicated an anisotropic magnetoresistance and an anomalous Hall effect.

Aim of the proposal:
The aim of the experiment was to investigate in a first step the magnon dispersion at T=10K along the high symmetry directions [001] and [100]. Such study could make an interesting case on how basic microscopic knowledge could help us understand and design materials for applications.

Experimental setup:
IN22 was set up in W-configuration. We used a double focusing PG monochromator, a PG analyzer and a PG filter in the neutron scattered beam. The data have been collected with a fixed k_f=2.662Å^{-1}. The single crystal (with a mass of about 10g) was mounted with the [100] – [001] directions in the scattering plane. An orange cryostat was used to cool the sample at base temperature.

Results:
Inelastic neutron scattering measurements on IN22 were mainly performed at T=10K. Few scans were repeated at high temperatures, i.e. 317K, in order to confirm the magnetic nature of the measured excitations. In order to extract the magnon branches, energy scans at constant q and q-scans at constant energies were performed along the directions [h 0 0] and [0 0 l]. Before fitting, every spectrum was analyzed carefully looking for spurions, in particular Aluminum contamination, and the corresponding regions were cut out. Gaussian functions were used to fit the observed peaks. Some characteristic q-scans at constant energies with the corresponding fits along the [0 0 l] direction are shown in Fig.1. Fig.2 shows the preliminary magnon dispersion of Mn_5Ge_3 along [00l] at T=10K.

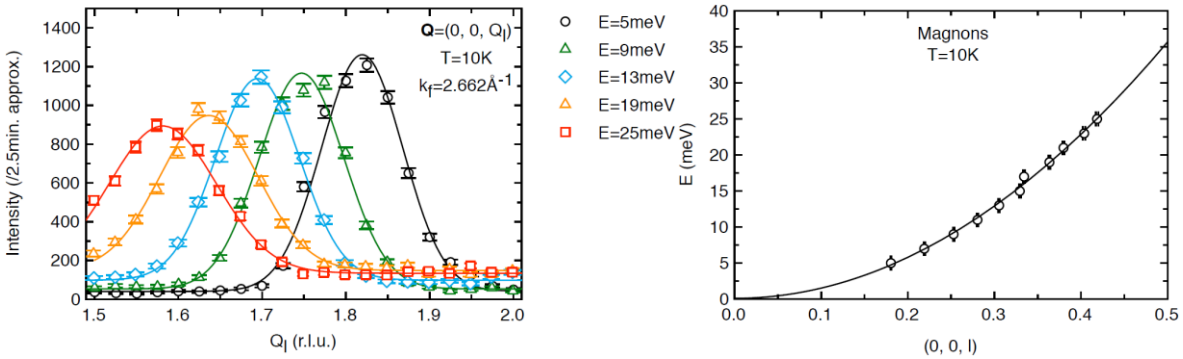

Fig.1 (left): Q_l-scans measured around **Q**=(002) at T=10K. The solid lines indicate fits with Gaussian functions.
Fig.2 (right): Preliminary magnon dispersion of Mn_5Ge_3 along [00l] at T=10K. Line is guide for the eyes.