Experimental report

06/09/2022

Proposal:	**5-54-325**
Council:	10/2019
Title:	Magnetic structure of Mn2GaC by neutron diffraction
Research area:	Physics

This proposal is a new proposal

Main proposer: **Quanzheng TAO**

Experimental team: Navid QURESHI
Quanzheng TAO

Local contacts: Bachir OULADDIAF
Ketty BEAUVOIS

Samples: Mn2GaC

Instrument	Requested days	Allocated days	From	To
D10	10	8	10/02/2021	18/02/2021

Abstract:

Magnetic MAX phases are interesting for potential application in spintronics and as precursor for magnetic 2D materials. Mn2GaC is a prototype magnetic MAX phases, consisting of Mn2C layers interleaved with Ga layers. It shows two magnetic transitions at TN=507 K and Tc=220 K. We did neutron diffraction experiment on Mn2GaC thin film sample along (00L) direction at HB1A at ORNL and Super Adam at ILL. The results suggest that the propagation vector is incommensurate with a small component along a* and/or b*. We propose to study the magnetic structure with D10 to scan the peak at Q=0.73 and Q=0.25 along a* and b* to determine the propagation vector, and then scan several peaks around (00L) and (10L) to refine the spin orientation. The sample is 10mm*10mm*100nm, epitaxially grown on MgO (111). Previous neutron diffraction experiments demonstrate the feasibility and magnetic Bragg peaks are comparable to (004) nuclear peak in intensity.

Magnetic structure of Mn_2GaC thin film by neutron diffraction with D10

MAX phases are a group of atomically laminated materials based on a transition metal (M) which can be partially substituted with a rare earth, an A-group element (A), and carbon or nitrogen (X), combining the characteristics of metal and ceramic [1,2]. MAX phases are promising materials for various applications, for example as precursor for 2D materials. Here we are interested in a magnetic MAX phase with M = Mn, which can potentially be used for spintronic applications or as precursor for magnetic 2D materials.

Mn_2GaC is a prototype magnetic MAX phase. The structure of Mn_2GaC (space group $P6_3/mmc$) consists of Mn_2C layers interleaved with Ga layers. The competition between antiferromagnetic and ferromagnetic interactions within the Mn_2C planes gives rise to complex magnetic behaviors. Mn_2GaC orders magnetically below $T_N = 507$ K and shows another magnetic transition at $T_C = 220$ K. The second transition is accompanied by a huge contraction of the *c* lattice parameter. First principles calculations predicted a canted antiferromagnetic structure, with $\mathbf{q} = (0, 0, 1/2)$ [3]. A schematic is shown in Fig. 1a. Figure 1b shows the magnetization vs. applied magnetic field at different temperatures. The magnetic structure has yet to be determined experimentally.

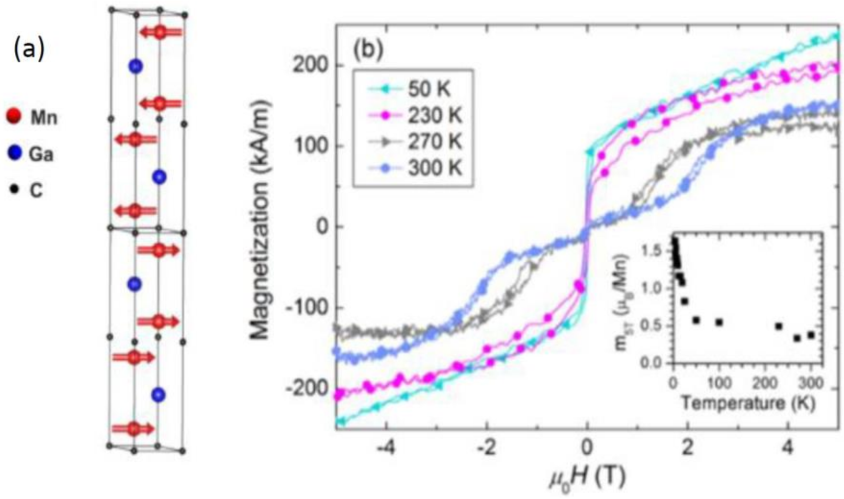

Figure 1. (a) Schematic magnetic and crystal structure of Mn_2GaC [3]. (b) Magnetization of Mn_2GaC with $H \parallel ab$ at different temperatures [4].

To understand the complex magnetic behavior of Mn_2GaC, a determination of its spin structure is needed. We initiated experimental investigations of the magnetic structure by neutron diffraction on D10 and Super Adam at ILL. We used a thin film grown parallel to (001) and scanned along the (0, 0, L) direction. At T = 3 K, peaks were observed at incommensurate positions $(0, 0, L) + \mathbf{q}_1$, with $\mathbf{q}_1 \approx (0, 0, 0.55)$ and L = even, as shown in Fig 2a. Fig 2bc show H and K scans for the reflection with $L \approx 3.45$. Narrow peaks centering at H=0 and K=0 indicate that there is no off-axis component of $\mathbf{q}_1$.

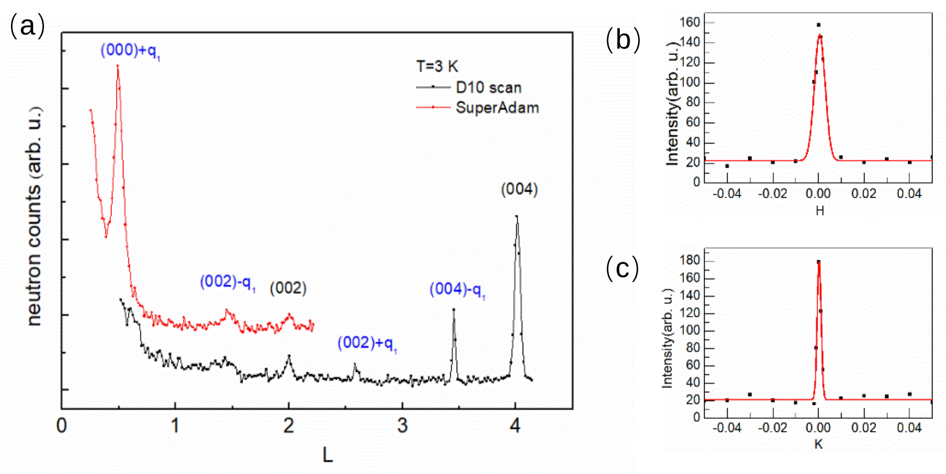

Figure 2. (a) Neutron diffraction measured with Super Adam and D10 at ILL. (b,c) H and K scan of the $(004) - \mathbf{q}_1$ reflection.

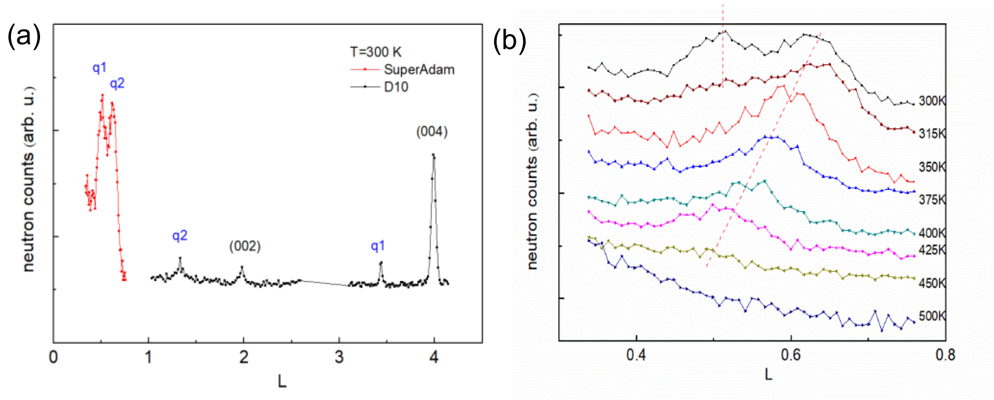

Figure 3. (a) Neutron diffraction at 300 K. Two propagation vector are present. (b) Temperature evolution of the diffraction intensity around L ~ 0.5.

Figure 3a shows the neutron diffraction at 300 K. As well as the reflections belonging to $\mathbf{q}_1$, another set of reflections belonging to $\mathbf{q}_2 = (0, 0, 2/3)$ are present. Figure 3b shows the temperature evolution of the intensity around L = 0.5. A peak at L ≈ 0.5 appears below 425 K. With decreasing temperature, the peak moves to higher Q, splits into two at about 315 K, the two peaks moves towards each other, and finally a single peak emerges at 3 K.
After symmetry analysis, the following three magnetic models are proposed as shown in table 1. To uniquely identify the magnetic model, further experiments covering 10*l* peaks are planned during October 2022.

Table1. Calculated intensity of reflections from different magnetic models.

Magnetic model	002 -q	004-q	100 -q	110 +q	102-q
Spiral	100	72	14	14	4
SDW [100]	100	72	28	25	8
SDW[120]	100	72	0	1	1

[1] Q. Tao *et al.,* Nature communications **8**, 14949 (2017) [2] Q. Tao *et al.*, Chemistry of Materials **31**, 2476 (2019)
[3] I. Novoselova *et al.*, Scientific Reports **8**, 2637 (2018) [4] M. Dahlqvist *et al.*, Phys. Rev. B **93**, 014410 (2016)
[5] A. Ingason *et al.*, Phys. Rev. B **94**, 024416 (2016) [6] H. Jonsson *et al.*, Phys. Rev. B **105**, 035125 (2022)