Magnetic structure of Mn_2GaC thin film (MAX phase) – ^{55}Mn Nuclear Magnetic Resonance Study

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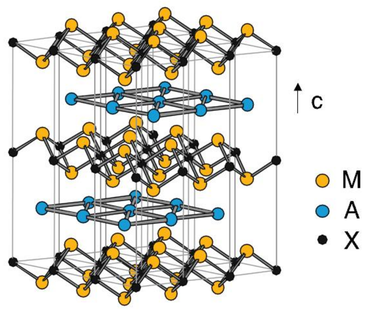
MAX phases - Background and Motivation

$M_{n+1}AX_n$, (n = 1-3)



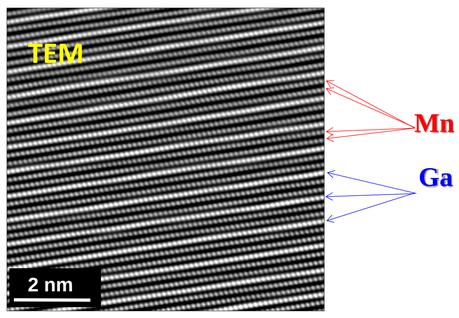
Schematic arrangement of atoms in the M_2AX compound

Mn_2GaC ternary compound belongs to the rich family of materials, known as the MAX phases [1]. They are composed of the nanolaminated carbides and nitrides described by the general formula $M_{n+1}AX_n$ where M is a transition metal, A stands for an A-group element (mostly group 13 and 14), X denotes carbon or nitrogen and n can take the numbers 1, 2 or 3 . The different elements form individual atomic layers and the atomic planes of magnetic element alternate with those containing non-magnetic atoms.

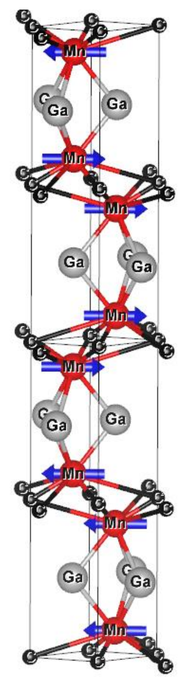
In order to control the complex magnetic behavior and to manipulate their properties, it is essential to understand the magnetic interactions between elements forming this quasi two dimensional structure. To this end, we performed the NMR study in presence of external magnetic field.

Mn_2GaC - Sample growth and structure

Mn_2 Ga C
Epitaxial films on MgO (111) substrate
thickness = 100 nm



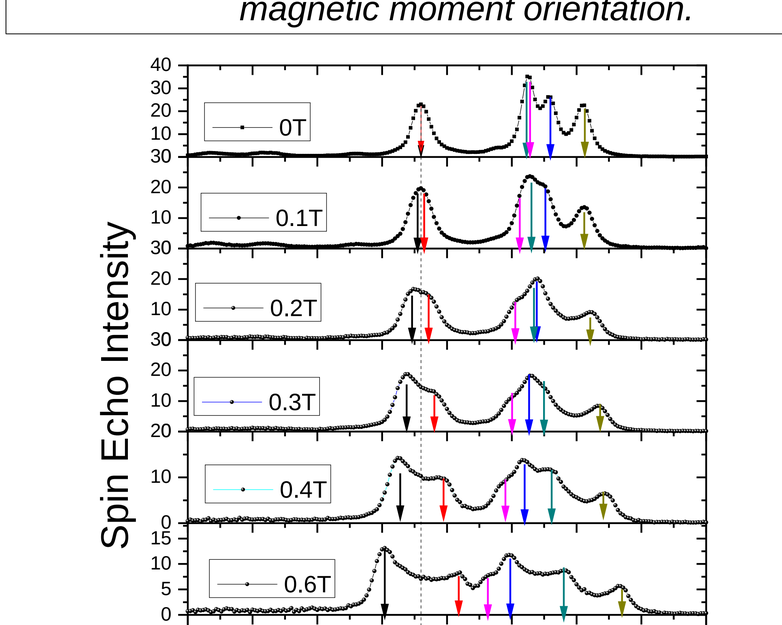
Symmetry group $P6_3/mmc$
Lattice parameters
a = 2.9 Å , c = 12.6 Å [2]



Mn_2GaC -
Neutron reflectometry
magnetic structure [3]

$AFM[0001]^A_4$
Long-range antiferromagnetic order:
- **1 Mn magnetic position**
- **Ferromagnetic** coupling accross carbon (C) layer
- **Antiferromagnetic** coupling **across every second A (Ga) layer**
- This structure has a **magnetic repetition distance of two unit cells (25.1 A°).**

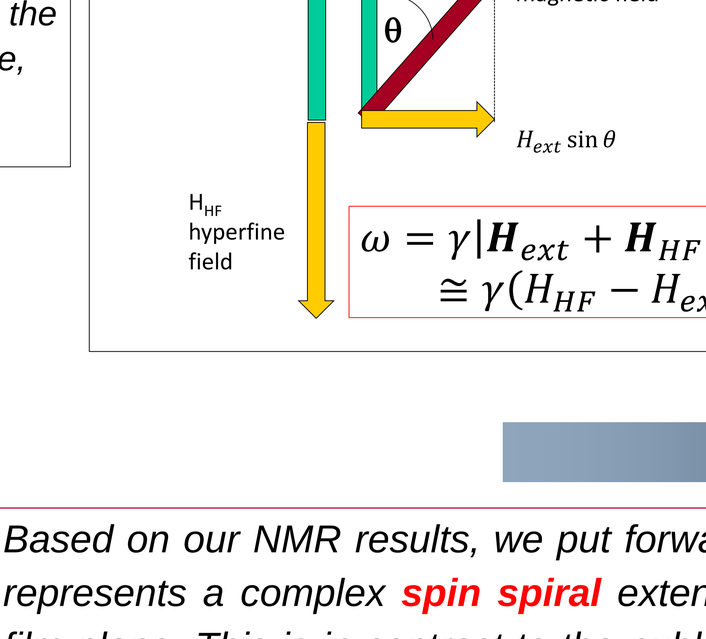
Mn_2GaC - ^{55}Mn, ^{69,71} Ga NMR spectra (zero external field)



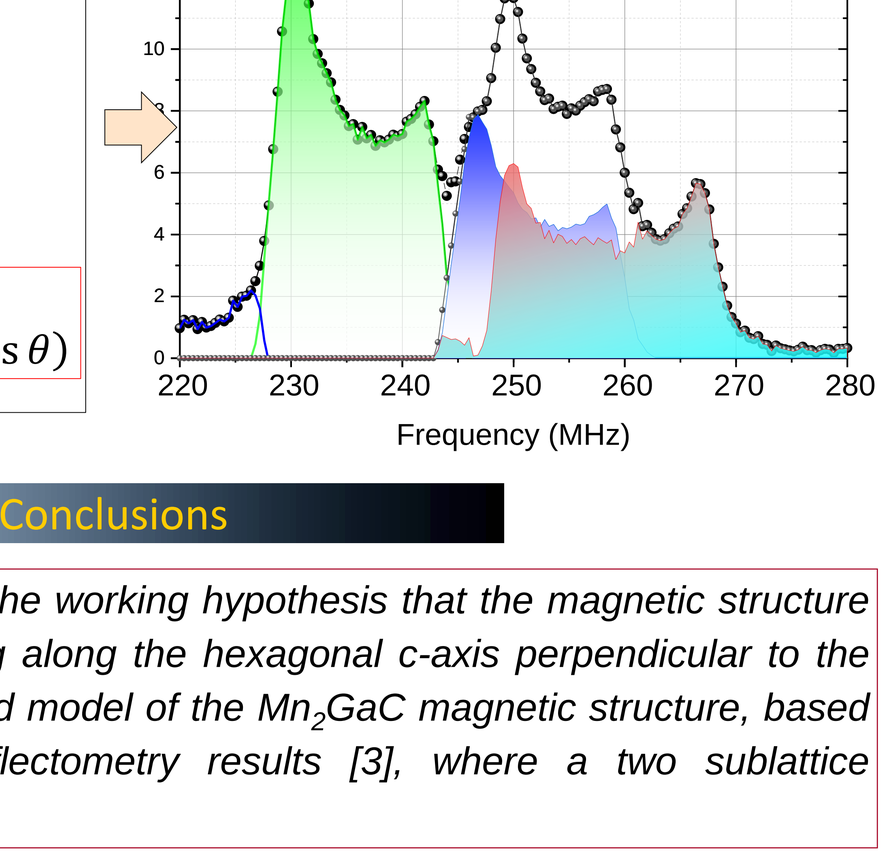
From zero field NMR
Four (4) ^{55}Mn hyperfine field values –
4 non-equivalent Mn magnetic positions
Hyperfine field : 22.36 T; 23.88 T; 24.26 T; 24.73 T
Magnetic moment: 1.86 μ_B; 1.99 μ_B; 2.02 μ_B; 2.06 μ_B;
One (1) ^{69,71}Ga hyperfine field value – one Ga position

Results

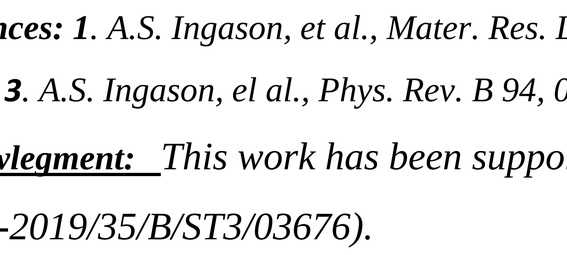
Mn_2GaC – magnetic structure deduced from ^{55}Mn NMR



Mn_2GaC - ^{55}Mn NMR frequencies as a function of external magnetic field applied in the film plane



Theory : NMR in external magnetic field



$$\omega = \gamma|\boldsymbol{H}_{ext} + \boldsymbol{H}_{HF}| \cong \gamma(H_{HF} - H_{ext}\cos\theta)$$

Mn_2GaC - ^{55}Mn NMR spectrum decomposition (in-plane external field H = 0,6T)

Mn_2GaC - *Evolution of the ^{55}Mn NMR spectrum: in the external magnetic field applied in the hexagonal plane, each ^{55}Mn NMR line reveals the distribution of Mn magnetic moment orientation.*

Conclusions

*Based on our NMR results, we put forward the working hypothesis that the magnetic structure represents a complex **spin spiral** extending along the hexagonal c-axis perpendicular to the film plane. This is in contrast to the published model of the Mn_2GaC magnetic structure, based of the DTF calculations and neutron reflectometry results [3], where a two sublattice antiferromagnet has been proposed.*

References: ***1***. *A.S. Ingason, et al., Mater. Res. Lett. 2, 89(2013),* ***2***. *I.P. Novoselova, et al., Scientific Reports 8, 2637 (2018),* ***3***. *A.S. Ingason, el al., Phys. Rev. B 94, 024416(2016).*

Acknowlegment: *This work has been supported in part by a grant from NSC, Poland (UMO-2019/35/B/ST3/03676).*