Experimental report

02/10/2023

Proposal: **5-12-363** **Council:** 4/2023

Title: Origin of the magnetostrictive behaviour in a Ni-Mn-Ga-Co-In metamagnetic shape memory alloy single crystal

Research area: Materials

This proposal is a new proposal

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Samples: Ni43Mn31Co9Ga14In3

Instrument	Requested days	Allocated days	From	To
D3	6	6	30/05/2023	06/06/2023
D9	9	9	08/11/2023	17/11/2023
ORIENTEXPRESS	1	1		

Abstract:

Ni-Mn-based magnetic shape memory alloys, MSMAs, are active materials that undergo martensitic transformations induced by temperature, stress and/or magnetic fields. This lead to large recoverable mechanical transformations, due to either a reorientation of martensitic twin-variants or a magnetic-field induced martensitic transformation. Ni-Mn-Ga-Co-In alloys present a metamagnetic behaviour in their martensite phase, where stoichiometry controls the critical transformation temperatures: structural, TM, and magnetic, TC. It was shown that with an exact composition of Ni43Mn31Co9Ga14In3, the single crystal shows magnetic field dependant twin-variants making that composition extremely interesting for applications. Being these applications dependant on the atomic site occupancies and magnetic structure, and those influenced by the form of the material (polycrystal, single crystal, thin films), we propose to carry out a single crystal diffraction study with the goal of elucidating the role of the atomic site occupancies in a Ni43Mn31Co9Ga14In3 single crystal.

EXPERIMENT N°: 5-12-363 **INSTRUMENTS:** D3 (D9 in the future)

DATES OF EXPERIMENT: 30/05/2023 - 06/06/2023

TITLE: Origin of the magnetostrictive behavior in a Ni-Mn-Ga-Co-In-Fe Metamagnetic Shape Single Crystal

REPORT 28/09/2023

Among the family of active materials capable of undergoing a deformation in the presence of an external magnetic field, known as magnetostrictive materials, Magnetic Shape Memory Alloys (MSMAs) can be found. These materials are characterized by regaining their original shape after the removal of the applied magnetic field. This process happens as a result of the martensitic transformation, a first-order solid state transformation involving both structural and magnetic changes. Ni-Mn-Ga-based MSMAs allow this transformation to be controlled by tuning the composition, atomic order and structure.

In previous work (experiment 5-23-784, performed at D1B in ILL) the crystalline phases and atomic site occupancies of a series of Ni-Mn-Ga-Co-In-Fe polycrystalline alloys were studied. The goal was to elucidate the effect a 0 to 5 at.% Mn substitution with Fe has on both the hysteresis and structural and magnetic transition temperatures. In this line, this experiment 5-12-363 was proposed, with the aim of understanding the behavioral and structural difference between same-composition single crystal and polycrystal.

$Ni_{43}Mn_{31-x}Co_9Ga_{14}In_3Fe_x$ (x = 0 and 2) single crystals were analysed during the experiment performed at the single crystal neutron diffractometer D3 in its polarised neutron diffraction set-up. Several measurements were obtained in their austenitic phase at different temperatures: above (T1), close to (T2) and below (T3) the Curie temperature, so information about different magnetic states could be obtained. The composition, measurement temperatures and structural and magnetic transformation temperatures of both crystals are shown in Table 1.

Name	Composition	T_C	T_M	T1	T2	T3
Fe0	$Ni_{43}Mn_{31}Co_9Ga_{14}In_3$	590	475	650	560	510
Fe2	$Ni_{43}Mn_{29}Co_9Ga_{14}In_3Fe_2$	505	360	600	430	390

Table 1. Names and compositions of the two samples measured at D3 during the experiment, with the temperatures (in Kelvin) at which information was acquired and the structural (T_C) and magnetic transformation (T_M) temperatures.

Mag2pol was used to represent the magnetic sites distribution in the unit cell of each alloy, based on the acquired data. In the obtained image (Figure 1), the increase in the magnetic moment with the Fe doping can be seen, alongside with the presence of negative magnetic moment in the Fe-doped sample at those temperatures below Curie temperature. The explanation to this effect can be found extrapolating the Rietveld refinement performed on the same composition polycrystals. In that refinement, the conclusion of Fe dopant occupying manganese positions and interacting antiferromagnetically with manganese atoms was drawn.

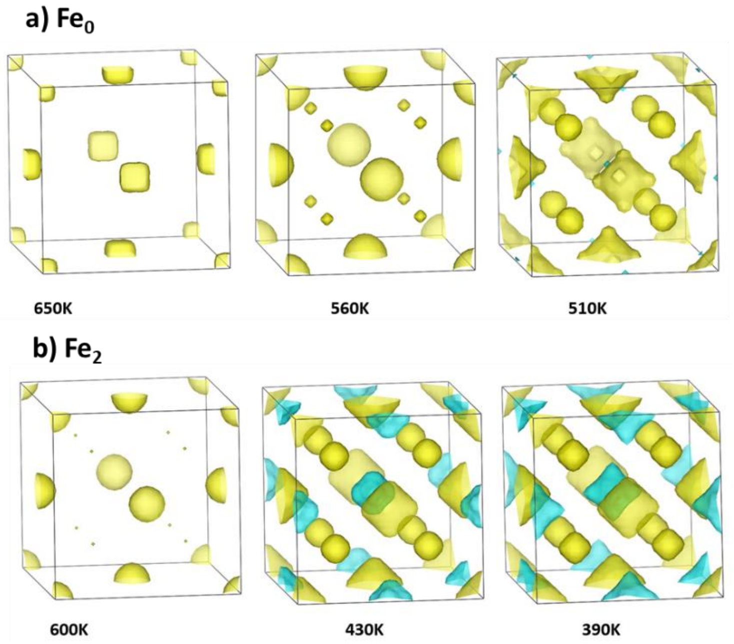

Figure 1: Magnetic moment distribution in the austenitic phases (Fm3m cubic structure) of the measured a)Fe_0 and b)Fe_2 alloys.

Further analysis will be done after the beamtime scheduled at D9 (08/11/2023 – 17/11/2023), when non-polarized neutron diffraction experiment will be performed in this set of single crystals, and structural information will be acquired.