Experimental report

25/10/2022

Proposal:	**5-14-271**		**Council:**	10/2019
Title:	Structure factors and magnetic moment distribution in a 6-element magnetic shape memory alloy single crystal			
Research area:	Materials			

This proposal is a resubmission of 5-14-267

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Samples: NiMnGaCoCuFe

Instrument	Requested days	Allocated days	From	To
D9	6	6	21/08/2020	27/08/2020

Abstract:

Mangetic Shape Memory Alloys are active materials that actuate mechanically upon the application of an external magnetic field. An attractive group of MSMAs are those with a large magnetic field induced strain (MFIS), with deformations up to 12%. This MFIS is possible by the large magnetic anisotropy energy of the variants and the magnetostatic coupling between lattice and spin, allowing manipulating the crystal structure by a magnetic field. Additionally, magnetic coupling between atoms will depend on their positions within the lattice. In this proposal we aim at completing the study of a single crystal of a MSMA composed of six different elements (NiMnGaCoCuFe), which was already measured in D3 under the EASY proposal number EASY-391. In order to determine the full atomic site occupancies and magnetic moments distribution in each site, previous information related to the nuclear structure is necessary in combination with the data obtained from D3.

EXPERIMENT N°: 5-14-271 **INSTRUMENTS:** D9

DATES OF EXPERIMENT 21/08/2020-27/08/2020

TITLE: Structure factors and magnetic moment distribution in a 6-element magnetic shape memory alloy single crystal

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Active materials are defined as those that are capable of changing at least one of their physical properties in the presence of external stimuli. Some of these active materials have a mechanical response to the pertinent stimulus, making them ideal candidates to be implemented as sensors or actuators. This mechanical response makes it possible to monitorize and control the properties of a more complex system where the active materials are part of it. Shape Memory Alloys (SMAs) are a group of active materials that undergo phase transitions (resulting in large recoverable mechanical deformations) induced by changing the temperature and/or applying a stress on them. When the actuation can be induced not only by temperature or stress, but also upon the application of an external magnetic field, the materials are named Magnetic Shape Memory Alloys (MSMAs). The properties shown by MSMAs, mainly the superfast response (in the millisecond regime) and the high energy density (of the order of 10^5 J/m^3), make them the ideal candidates to be implemented in the field of sensors and actuators.

The variant reorientation responsible of this actuation, generated at the martensitic transformation, is possible by the large magnetic anisotropy energy of the variants in the external field and the magnetoelastic coupling between lattice and spin, which allows manipulating the crystal structure by a magnetic field. The magnetic coupling between atoms, which depends on their positions within the lattice, and the magnetic moment distribution are therefore of the utmost importance for the properties of these materials.

In this experiment we have completed the study of a single crystal of a NiMnGaCoCuFe magnetic shape memory alloy. Measurements at 250 K, to measure the ferromagnetic martensite phase of the alloy, and at 540 K, to measure the paramagnetic austenite phase, have been performed. Initial fittings to the data have helped us to elucidate the nuclear form factors at each site in the paramagnetic austenite phase, whose Rietveld analysis yielded the atomic site occupancies depicted in Fig.1.

Estructura tipo $L2_1$

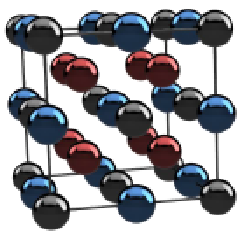
Grupo de simetría Fm-3m

Ocupaciones:

8c: (¼ ¼ ¼) y (¾ ¾ ¾)

4a: (0 0 0)

4b: (½ ½ ½)



Site (Wyckoff)	Ni	Mn	Ga	Fe	Co	Cu	Total
8c	1.81	0.12	0	0.07	0	0	2
4a	0	0.65	0	0.13	0	0.22	1
4b	0	0.03	0.76	0.02	0.19	0	1

Figure 1: Atomic site occupancies and symmetry group of the studied MSMA single crystal in the austenite phase, at 540K

A more detailed study of the martensite phase of the alloy, including a fine Rietveld refinement, is still pending.