Proposal:	EASY-391		<b>Council:</b> 4/2018			
Title:	The role of Fe addition on magnetic shape memory alloys: atomic distribution influence on magnetic coupling					
Research area: Materials						
This proposal is a new proposal						
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Experimental team:						
Local contacts:	Anne	Anne STUNAULT				
Samples: NiMnGaCoCuFe						
Instrument			Requested days	Allocated days	From	То
D3			24	24	26/10/2018	27/10/2018
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 studying the role of iron in the magnetic and structural properties of single crystals of MSMAs with significant differences in their compositions, with the objective of elucidating how the atomic site occupancy and magnetic moment distribution affect the structural and magnetic properties of the MSMAs in simple and complex (4 and 7 element alloys) structures. Due to the high differences between the Mn, Co and Fe neutron scattering length densities, a neutron diffraction experiment in the samples proposed for this experiment will allow us to unravel with precision the atomic site occupancies in each phase of the alloys.

## **EXPERIMENT N°:** EASY-391

## **INSTRUMENTS: D3**

## DATES OF EXPERIMENT 26/10/2018-27/10/2018

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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<sup>5</sup> J/m<sup>3</sup>), 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.

With this easy access proposal we measured the flipping ratios at different temperatures of a 6-element NiMnGaCoCuFe magnetic shape memory alloy, aiming at determining the magnetization density distribution in the MSMA single crystal (Fig.1), at the different crystallographic phases (ferromagnetic martensite below  $T_A$ , ferromagnetic austenite above  $T_A$  and below  $T_C$ , and paramagnetic austenite above  $T_C$ ).

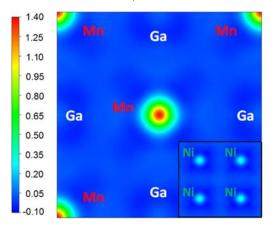


Figure 1: Preliminary magnetic moment distribution of the NiMnGaCoCuFe single crystal at x=0 (main) and x=0.25 (inset) planes measured in D3. The colour code units are  $\mu$ B/Å3. An approximate model has been used for the calculation of the nuclear structure factors needed for the determination of the magnetization density

The results obtained with this experiment will be cross-correlated with those obtained in the experiment 5-14-271, which is a single crystal non-polarized neutron diffraction experiment in

the same MSMA alloy, whose full analysis is still pending. The analysis of the data from D3 requires the measurement of the nuclear structure factors in similar conditions, together with the determination of the extinction correction. Once this analysis is done we will be able to unravel the magnetic site densities in the alloy studied by fully analyzing the data obtained in this experiment.