Experimental report

25/06/2018

Proposal: 5-31-2497 **Council:** 4/2016

Title: Investigation of modulated crystaland magnetic structure of Ni-Co-Mn-In Magnetic shape memory alloy

Research area: Physics

This proposal is a new proposal

Main proposer: Sanjay SINGH

Experimental team: Sanjay SINGH
Parul DEVI

Local contacts: Emmanuelle SUARD

Samples: Ni2Mn1.4In0.6
Ni1.8Co0.2Mn1.4In0.6

Instrument	Requested days	Allocated days	From	To
D2B	4	2	20/09/2016	22/09/2016

Abstract:

In the present work our aim is to investigate in detail the crystal and magnetic structures of the martensite phase in Ni2Mn1.4In0.6 and Ni1.8Co0.2Mn1.4In0.6 magnetic shape memory alloysas a function of temperature. These measurements will be done using neutron diffraction and will resolve the disagreement in literature about the magnetic structure of these compounds. Modulation introduces atomic displacements, which must be correlated with the magnetic properties. Therefore, a complete structural study of Ni2Mn1.4In0.6 and Ni1.8Co0.2Mn1.4In0.6 magnetic shape memory alloys taking into account the complex interplay between incommensurate nuclear and magnetic structure will be done.

Investigation of modulated crystal and magnetic structure of Ni-(Co)-Mn-In magnetic shape memory alloy

Experimental report: 5-31-2497 (D2B)

The aim of the experiment was to investigate the crystal and magnetic structure of $Ni_2Mn_{1.4}In_{0.6}$ and $Ni_{1.8}Co_{0.2}Mn_{1.4}In_{0.6}$ magnetic shape memory alloys as a function of temperature in the both austenitic and martensitic phases. The origin of incommensurate structural modulation in Ni-Mn based Heusler type magnetic shape memory alloys (MSMAs) is still an unresolved issue. Two different models have been proposed in the literature for the origin of modulation in the MSMAs. The first one is the adaptive phase model, which consider the modulated structure as a nanotwinned state of the Bain distorted phase, which maintains the invariance of the habit plane between the high temperature austenite and the low temperature martensite phases. Commensurate modulated structure, uniform atomic displacements and absence of any premartensite phase transition as well as phason strains are important signature of this model. On the other hand, the second model, known as soft phonon mode model, a non-uniform atomic displacement, incommensurate nature of modulation and existence of premartensite phase as well as phasons are proposed. However,

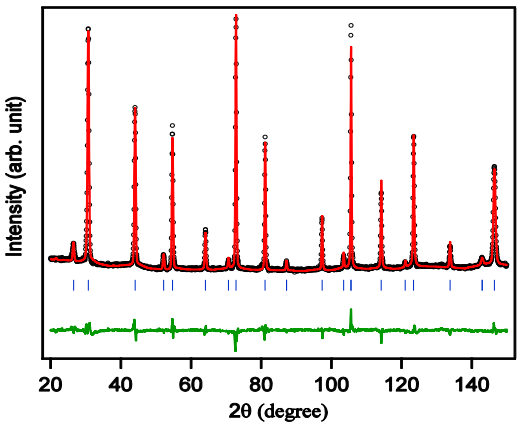

Fig.1: The observed (black circles) and calculated (red line) neutron powder diffraction pattern at 300 K (austenite phase). The lower (green) curve shows the difference. The blue ticks are Bragg peaks position.

discommensurations in the form of stacking faults and antiphase boundaries can in principle result into an average incommensurate modulated structure even for the adaptive phase model. Therefore, one of the important feature to separate between these two models is the identification of the nature (uniform versus non-uniform) of the displacement of atoms from their mean position. The neutron diffraction measurement on these smples were carried out at D2B with λ= 1.6 Å in the 2θ range 0-160^0 in steps 0.05^0.

The results of Rietveld refinement using the neutron powder diffraction pattern of $Ni_2Mn_{1.4}In_{0.6}$ at

300 K (RT) in the austenite phase is shown in Fig. 1. The refinement was done by considering the atomic positions within the Fm-3m space group. The Ni and Mn atoms occupy the 8c (0.25 0.25 0.25) and 4a (0 0 0) Wyckoff positions, respectively, while In and extra Mn occupy the 4b (0.5 0.5 0.5) Wyckoff positions according to their relative occupancies. In the refinement, we also considered the possibility of anti-site disorder between different atoms (atomic sites) (e.g Ni(8c)-Mn(4a), Mn(4a)-In(4b) and Ni(8c)-In(4b)) but could not observe any improvement in the fits or the agreement (R) factors. Therefore, the analysis of the Rietveld analysis of RT neutron diffraction data confirms absence of any substantial anti-site disorder in $Ni_2Mn_{1.4}In_{0.6}$ alloy.

Next, we performed the refinement of the martensite structure. The neutron diffraction data for the martensite phase was collected at the lowest possible temperature (3K). To investigate the modulated structure, we employed superspace (3+1) D formalism. Initially the refinement was carried out without any constraints on the amplitude or direction of atomic displacements for the atomic modulation functions of the different atoms as expected in the soft phonon mode model but it led to unreasonable interatomic distances (Fig.2a).

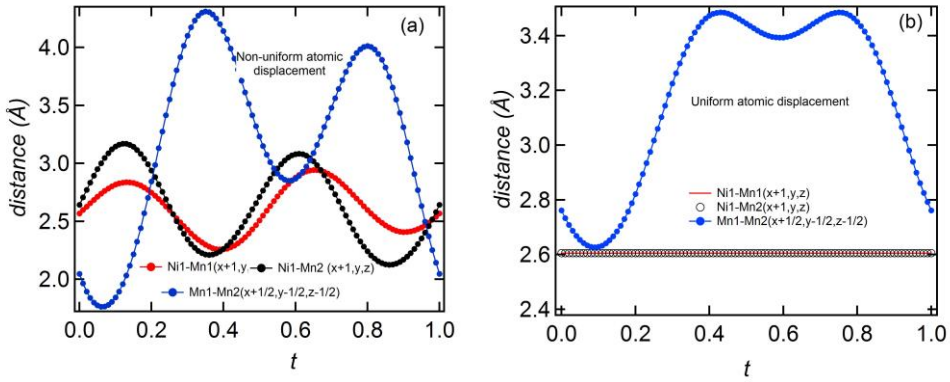

Fig.2: Distance (selected) as a function of *t* parameters derived from (a) Non-uniform atomic displacement model (soft phonon mode model) showing unphysical values (less than 2.5Å) and (b) Uniform atomic displacement model (adaptive phase model) showing values that are expected for these kinds of intermetallic alloys.

In the next step, we therefore considered a uniform displacement model for Rietveld refinement in which the amplitude of modulation for all the atomic sites was constrained to be identical. This model gives physically realistic interatomic distances (Fig.2b) that are acceptable for the shape memory Heusler alloys. Thus, our results based on both PND reveal that the modulation in the martensite phase of $Ni_2Mn_{1.4}In_{0.6}$ involves uniform displacement of atoms and is, therefore, consistent with the predictions of the adaptive modulation model. We have also confirmed the applicability of adaptive phase model using high resolution synchrotron x-ray diffraction study. Results of experiments done on this proposal are published in **Phys. Rev. B 97, 224102 (2018) and** another work is in under review **(**arXiv:1806.05075v1**).**