Experimental report

01/06/2016

Proposal: 5-31-2368 **Council:** 10/2014

Title: Magnetic and crystal structure of Ni-Pt-Mn-Ga ferromagnetic shape memory alloys by powder neutron diffraction

Research area: Physics

This proposal is a new proposal

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Samples: Ni1.9Pt0.1MnGa

Instrument	Requested days	Allocated days	From	To
D2B	4	2	06/07/2015	08/07/2015

Abstract:

In the present work our aim is to investigate the magnetic and crystal structure of new Pt doped Ni2MnGa (Ni-Pt-Mn-Fa) ferromagnetic shape memory alloys as a function of composition and temperature. The measurements will be done using neutron diffraction technique, which will give valuable new input to understand their structural and magnetic property and disorder effects. The high resolution neutron diffraction measurement in the premartensite and martensite phases will provide the nature and degree of modulation, which is an important factor, which determines the magnetic field induced strain in Ferromagnetic shape memory alloys.

Magnetic and crystal structure of Ni-Pt-Mn-Ga ferromagnetic shape memory alloys by powder neutron diffraction

It was proposed to investigate the magnetic and crystal structure of Pt doped Ni_2MnGa (Ni-Pt-Mn-Ga) ferromagnetic shape memory alloys as a function of composition and temperature. From magnetic measurements it was found that with increasing Pt in Ni_2MnGa the magnetization decreases. The neutron measurements were expected to give valuable new input to understand the magnetic property of these alloys and its relation to the disorder effects. The neutron diffraction measurement on these samples were carried out at D2B with λ= 1.6 Å in the 2θ range 0-160^0 in steps 0.05^0.

Results

The magnetism of Mn-based Heusler alloys is mainly governed by Mn, which has been observed experimentally and shown by *ab initio* calculations for these systems. However, the magnetization may change dramatically due to disorder. Therefore, to study the origin of the large magnetization drop observed in NiPtMnGa, we performed neutron diffraction measurements and analyzed the data using the Rietveld refinement procedure (Fig. 1). In the first step of the refinement, we follow the LeBail fitting procedure using the tetragonal unit cell with SG *I4/mmm*. This model could index all the Bragg reflections confirming that NiPtMnGa exhibits the tetragonal structure at RT. In the next step, we performed the Rietveld refinement, by taking into account the atomic positions and occupancies of the atoms within the unit cell. Mn(2*a*)/Ga(2*b*) antisite disorder. The initial atomic positions were taken as Ni(4*d*) and Pt(4*d*), Mn(2*a*), and Ga(2*b*) [Fig. 2(a)]. Here, 4*d*, 2*a*, and 2*b* are the Wyckoff positions in the tetragonal unit cell. The nuclear scattering amplitudes for Ni, Mn, and Ga (10.3, −3.73, and 7.23 fm, respectively) are very distinct, which allows the determination of the actual atomic occupancies and the antisite disorder present in NiPtMnGa. Both fits, without and with Ni(4*d*)/Mn(2*a*) disorder are unsatisfactory

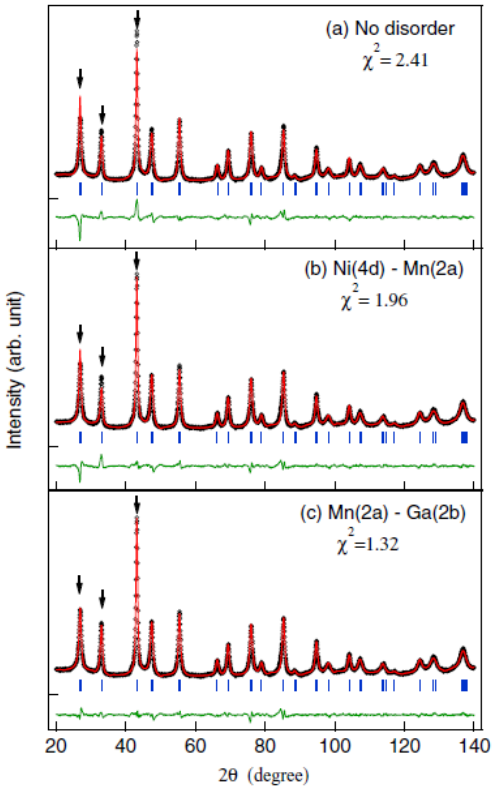

Fig.1: Rietveld refinements of powder neutron diffraction pattern of NiPtMnGa at RT. The observed patterns (black circles) have been fitted (red solid lines) assuming (a) no disorder, (b) Ni(4d)/Mn(2a) disorder, and (c) Mn(2a)/Ga(2b) antisite disorder. The vertical arrows indicate the (101), (110), and (112) Bragg peaks (from left to right, respectively) of the tetragonal unit cell (SG I4/mmm). The green curve shows the difference between the measured and refined patterns. The vertical ticks are the Bragg peak positions.

[χ2 = 2.41, 1.96, respectively, see Figs. 1(a) and 1(b)]. However, if the antisite Mn(2*a*)/Ga(2*b*) disorder is taken into account, we obtain a much better fit [χ2 = 1.32, Fig. 1(c)]. The tetragonal unit cell with Mn(2*a*)/Ga(2*b*) antisite defect is shown in Fig. 2(b). The refined site occupancies listed in Table I reveal about 17% of the Mn(2a)/Ga(2b) antisite disorder.

Table-1: Parameters obtained from the Rietveld refinement of the neutron diffraction pattern for NiPtMnGa at RT.

SG	$I4/mmm$		
Lattice parameters	$a = b = 3.964$ Å,	$c = 6.826$ Å	
Wyckoff site	4*d*	2*a*	2*b*
Pt occupancy	0.5	0	0
Ni occupancy	0.5	0	0
Mn occupancy	0	0.873(2)	0.163(2)
Ga occupancy	0	0.163(2)	0.873(2)

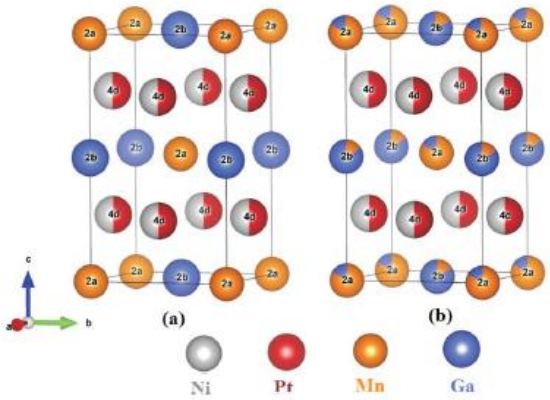

Fig.2: Tetragonal unit cell (SG I4/mmm) of NiPtMnGa with (a) no antisite disorder and (b) Mn(2a)-Ga(2b) antisite disorder. 2a, 2b, and 4d represent the crystallographic Wyckoff positions within the tetragonal unit cell.

Above mentioned results are published in S. Singh et al. Phys. Rev. B 93, 134102 (2016) [DOI: 10.1103/PhysRevB.93.134102]. For other compositions the analysis and manuscript preparation is in progress.