

Neutron diffraction study on the magnetic structure of $(\text{Fe}_{0.90}\text{Cr}_{0.03}\text{Ni}_{0.07})_2\text{P}$

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Abstract

Crystal and magnetic structures of $(\text{Fe}_{0.90}\text{Cr}_{0.03}\text{Ni}_{0.07})_2\text{P}$ have been investigated using neutron powder diffraction measurements over a temperature range of 10–300 K. The system crystallizes in Fe_2P type hexagonal structure ($P6_2m$ space group, $Z=3$) in which Cr atoms occupy the pyramidal Fe_{II} site and Ni atoms occupy the tetrahedral Fe_{I} site with total preference. Refined values of the cell parameters and atomic positional parameters are quite close to those reported for the parent compound Fe_2P . The substituted alloy retains the ferromagnetic order of Fe_2P with the moments orienting along $[001]$ direction. There are signatures of the presence of magnetic clusters. The ordered magnetic moments at 10 K are $0.88(2)\mu_{\text{B}}$ and $2.16(5)\mu_{\text{B}}$ at the two metallic sites Fe_{I} and Fe_{II} , respectively. These values are close to those reported for Fe_2P at 77 K. At 297 K, which is in the region of ferromagnetic to paramagnetic transition, the moment at Fe_{I} site is quite low at $0.14(3)\mu_{\text{B}}$ but at Fe_{II} site, it is still fairly large at $0.67(15)\mu_{\text{B}}$.

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1. Introduction

Fe_2P is one of the most interesting and complex magnetic materials in the transition metal metalloid systems with a subtle balance of ferromagnetic and anti-ferromagnetic exchange interactions [1–10]. Low level substitution for Fe by Ni in Fe_2P strengthens the ferromagnetic ordering. All the compounds in the series $(\text{Fe}_{1-x}\text{Ni}_x)_2\text{P}$ up to $x=0.50$ are ferromagnetic. With initial substitutions of Ni, T_{C} increases sharply [2–4]. As against a value of 216 K for Fe_2P , T_{C} values for Ni substitutions corresponding to $x=0.01$ and 0.05 are ~ 235 and 295 K, respectively [4]; for $x=0.08$, T_{C} is maximum at ~ 342 K [3]. Magneto-crystalline anisotropy decreases with introduction of Ni for Fe [3]. Mössbauer studies showed that for low level substitutions Ni preferentially occupies the tetrahedral site and the hyperfine fields at both the crystalline sites reduce [4,5]. Our previous

studies on 7% Ni substituted alloys showed that T_{C} is ~ 300 K and the saturation moment is comparable with that of Fe_2P [6]. It is further noted that introduction of Ni raises T_{C} but the values of the moments at the two metallic sites do not change much, vis-à-vis Fe_2P and the moments continue to orient along $[001]$ as in the parent compound Fe_2P [6]. It has also been established that introduction of Cr for Fe, in Fe_2P , destroys the ferromagnetic order; also there is a drastic decrease in T_{C} as well as in the magnetic moments at the two metallic sites [1,7]. In fact our studies on 3% Cr substituted system have shown that over a range of temperature from 300 down to 5 K the alloy exhibits four different kinds of magnetic behaviour [8].

In light of this unusually strong sensitivity of the substitutions of Ni and Cr for Fe in Fe_2P , it is of interest to examine the effect of simultaneous substitutions of Cr and Ni. The idea is to examine the effect on the magnetic properties of Fe_2P , of the substitution of one element tending to strengthen ferromagnetism and of another one tending to set in anti-ferromagnetism. Ghose et al. [9] reported magnetization and ac susceptibility measurements on two samples, viz., $(\text{Fe}_{0.90}\text{Cr}_{0.05}\text{Ni}_{0.05})_2\text{P}$ and $(\text{Fe}_{0.90}\text{Cr}_{0.03}\text{Ni}_{0.07})_2\text{P}$. The two alloys crystallize in Fe_2P type

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hexagonal structure and their lattice parameters are comparable to those of Fe_2P . It was inferred that the two alloys are ferromagnetic in nature (with $T_c = 180$ and 250 K, respectively). Subsequently, Srivastava et al. [10] investigated wait time dependence and ageing behaviour in the alloy $(\text{Fe}_{0.90}\text{Cr}_{0.05}\text{Ni}_{0.05})_2\text{P}$ using SQUID magnetometry and ac susceptibility measurements. The results confirmed a re-entrant spin glass phase in the system $(\text{Fe}_{0.90}\text{Cr}_{0.05}\text{Ni}_{0.05})_2\text{P}$.

In the present work, we have undertaken magnetization and neutron diffraction studies on the details of magnetic structure of the alloy with the other composition, viz., $(\text{Fe}_{0.90}\text{Cr}_{0.03}\text{Ni}_{0.07})_2\text{P}$, with simultaneous substitutions of Cr and Ni which have opposing effects vis-à-vis strength of ferromagnetic exchange.

2. Experimental details

The alloy $(\text{Fe}_{0.90}\text{Cr}_{0.03}\text{Ni}_{0.07})_2\text{P}$ (hereafter referred to as FCN37) has been prepared using the technique of solid state diffusion as described in reference [9]. High purity Fe powder (4N), Ni powder (4N), Cr pieces (4N) and red P flakes (5N) were used as the starting materials.

Powder X-ray diffraction (XRD) measurements using Mn filtered monochromatic Fe $K\alpha$ radiation ($\lambda = 1.937355$ Å) were made in the 2θ range of 3° – 100° on the Philips make X-ray powder diffractometer (model PW1840). A silicon sample (cubic with $a = 5.431$ Å in plate form) was used as a standard sample for internal calibration. The patterns have been analyzed and indexed with the help of Calligaris and Germa's Powder diffraction Package (PDP 11.1) [11].

Magnetization has been recorded on a SQUID magnetometer (Quantum design, MPMS) as a function of temperature down to 5 K in zero field cooling (ZFC) and field cooling (FC) modes in an external field of 25 Oe. For measurements in ZFC mode, the sample was cooled down to 5 K in zero field and then a magnetic field of 25 Oe was applied and magnetization was recorded as a function of temperature in the warming cycle from 5 to 296 K. For measurement in the FC mode, the sample was cooled down to 5 K in a field of the same strength (25 Oe) and magnetization was recorded in the cooling cycle. In addition to these measurements, magnetization–temperature data in the temperature range 90–315 K in a field of 50 Oe, and magnetization–field data at 90 K have also been recorded on a vibrating sample magnetometer (VSM).

Temperature dependent neutron diffraction (ND) measurements have been made on the sample in powder form at the 100 MW 'Dhruva' reactor at Bhabha Atomic Research Centre, Mumbai. Diffraction patterns have been recorded on a position sensitive detector based powder diffractometer [12,13]. Neutron beam of wave length $\lambda = 1.094$ Å has been used in all the experiments. For low temperature measurements down to 10 K, a closed helium cycle refrigerator (CCR) cryostat was used. For room temperature (297 K) measurements, ~ 10 g powder sample was packed in cylindrical vanadium container which was then loaded on the diffractometer in air. The room temperature patterns have been recorded in the 2θ range of 10° – 80° .

For low temperature measurements, the powdered sample was packed in an aluminum sample holder (for ensuring good thermal conductivity and less incoherent scattering). The only problem with aluminum is that its diffraction peaks may interfere with those of the sample. This aspect has been taken care of during profile refinement of the diffraction patterns. The sample holder was attached to the cold finger of an evacuated closed helium cycle refrigerator cryostat. Low temperature patterns have been recorded in the 2θ range of 10° – 40° .

ND patterns have been recorded at 10, 40, 80, 120, 230 and 297 K. Rietveld profile refinements of the ND patterns were carried out using the FULLPROF Program [14], where the magnetic part of the diffraction pattern can be treated as an additional 'phase'. In the nuclear structure refinement the parameters varied were: two cell parameters, two atomic positions, site occupancies, overall isotropic temperature factor in addition to the instrumental parameters such as zero angle, three half width parameters and a scale factor. From the observed pattern the background points corresponding to different angles have been directly fed as input. The profile shape has been taken as Gaussian function and a peak asymmetry correction was made for 2θ below 25° . The nuclear scatter-

ing lengths used in the analysis are: $b_{\text{Fe}} = 9.45$ fm, $b_{\text{Ni}} = 10.3$ fm, $b_{\text{Cr}} = 3.635$ fm and $b_{\text{P}} = 5.13$ fm.

For determination of the magnetic structure, low temperature diffractograms (i.e., in the magnetic state) have been analyzed using magnetic profile refinement method, in which the magnetic phase was treated as a second phase in addition to the nuclear phase. In the magnetic refinement, site occupancies obtained from the analysis of the 297 K pattern were kept constant and in addition the magnetization for the two metallic sites has been refined. The form factors corresponding to different ions have been taken from the paper of Watson and Freeman [15] and directly fed in to the refinement program.

3. Results and discussion

3.1. Characterization and crystal structure

All the peaks in the XRD pattern were indexed in Fe_2P type hexagonal symmetry; no other peak was detected from any other phase. This confirms single phase nature of the prepared alloy. In neutron diffraction measurements, however, we have observed two very weak reflections, almost merged in the background, which could not be indexed into Fe_2P like hexagonal symmetry. They could be identified as belonging to the Fe_3P phase which is reported to be ferromagnetic with $T_c = 686$ K [16]. However, as such, since the Bragg peaks of Fe_3P have only negligible overlap with the Fe_2P type pattern [17], these even otherwise weak impurity lines, do not constitute any hindrance in the determination of magnetic structure of FCN37. Also intensities of the parasitic reflection from Fe_3P remain nearly unchanged with temperature. The cell parameters were finally refined with the help of a least square refinement program. The obtained cell parameters are $a = 5.889(2)$ Å and $c = 3.474(2)$ Å, respectively which are close to those reported for Fe_2P [18].

3.2. Magnetic structure

3.2.1. Magnetization measurements

Fig. 1 shows temperature dependence of magnetization (M), in the temperature range 5–296 K, in ZFC and FC modes in an external field of 25 Oe. These measurements have been made on SQUID magnetometer. It is noted that in the ZFC mode, moment continuously increases in going from a temperature of 5 up to ~ 275 K and then it drops. In FC mode the magnetization is constant in the region between 5 and ~ 270 K and then it drops. The large difference in the ZFC and FC modes is indicative of magnetic relaxation. However, these curves, limited to ~ 295 K, do not fully exhibit magnetic transition. For locating the transition, we have plotted, in Fig. 2, M versus T in the range 90–315 K as recorded in the FC mode on VSM in an external field of 50 Oe. Brillouin curve appearance of this M – T curve is indicative of ferromagnetic to paramagnetic transition at $T_c \sim 295(5)$ K.

Fig. 3 shows field dependence of the magnetization at 93 K. This plot shows that the magnetization continuously increases with field but does not get saturated up to a field of 6.5 kOe. The moment at this field and temperature is ~ 73 emu/g which is more than the reported values for Fe_2P and $(\text{Fe}_{0.93}\text{Ni}_{0.07})_2\text{P}$ [6]. This observation, coupled with our inference, from the study of $(\text{Fe}_{0.93}\text{Ni}_{0.07})_2\text{P}$, that introduction of Ni for Fe in Fe_2P causes reduction in magneto-crystalline anisotropy, implies that addi-

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