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NEUTRON DIFFRACTION STUDIES OF $MnFeAs_yP_{1-y}$ SYSTEM

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Magnetic structures of the $MnFeAs_yP_{1-y}$ system were examined by means of the neutron diffraction technique in the 1.5–300 K temperature range. Atomic ordering in the metal sublattices, temperature dependence of the incommensurate ($y = 0.2$ and $y = 0.275$) and of the ferromagnetic ($y = 0.275$, $y = 0.3$, $y = 0.5$) ordering is discussed.

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1. Introduction

Structural and magnetic studies of the $MnFeAs_yP_{1-y}$ system of solid solutions have been performed for several years [1–4]. As a function of compositions, this system exhibits three different type crystallographic structures. For low As contents the compounds crystallize within the orthorhombic Co_2P type structure but for high As contents the tetragonal one of Fe_2As type structure was established. For composition range of $0.2 < y < 0.66$ the hexagonal structure of Fe_2P type was proposed.

From the magnetic point of view the most interesting properties, for samples within this intermediate composition range, were found. When the phosphorus atoms were substituted by arsenic atoms, it was observed that either the antiferromagnetic order ($0.2 < y < 0.26$) or ferromagnetic one ($0.26 < y < 0.66$) exist.

It is worth noting that for the $MnFeAs_yP_{1-y}$ system different first-order magnetic transitions induced by the high magnetic field were found. The deduced H–T phase diagrams show the evidence of the isolated or/and critical end points.

2. Experiment

To our knowledge, up till now, no magnetic structure determinations for this system are available in the literature. The polycrystalline samples with $y = 0.2$, $y = 0.275$, $y = 0.3$ and $y = 0.5$ have been chosen to analyze the magnetic structure evolution both as a function of composition and temperature (1.5 to 300 K).

The neutron diffraction experiments on the reactor at ILL, Grenoble were performed. To collect the diffraction patterns the D1B spectrometer was used.

For the numerical data analyses and for the magnetic structure determination two programs, ABF-Fit and MXD, respectively, from the VAX computer library were used.

3. Results and discussion

All the structure refinement performed in the *paramagnetic* state show that the (As, P) atoms are distributed in a disordered way, nevertheless a systematic reverse crystallographic ordering effect is observed between two metal sublattices. It means that small amount of the manganese atoms is substituted by the iron ones, in the pyramidal sites. This conclusion is strongly supported by the Mössbauer effect studies [1]. The spectra recorded for $MnFeAs_{0.5}P_{0.5}$ (room temperature, only) clearly show the evidence that the iron atoms are both present at the pyramidal and tetrahedral sites.

For the sample with $y = 0.2$ and with $y = 0.275$ the *incommensurate* magnetic structure takes place in the given ranges of temperature (Figs. 1 and 2). In

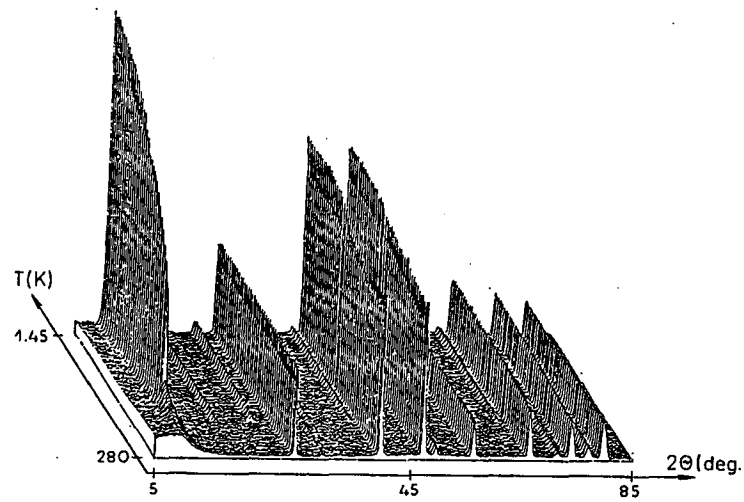

Fig. 1. The 3D neutron diffraction pattern for the $MnFeAs_{0.2}P_{0.8}$ recorded from 1.45 to 280 K.

any case, the manganese moments are disposed in a helicoidal configuration which propagates along the b^* direction. On the other hand, concerning the iron ones,

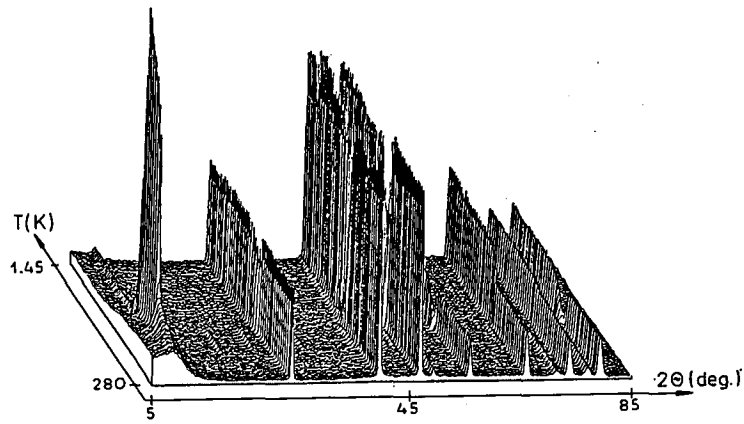

Fig. 2. The 3D neutron diffraction pattern for the $MnFeAs_{0.275}P_{0.275}$ recorded from 1.45 to 280 K.

they are oscillating along the same propagation direction, the easy sine axis being the c direction. It is worth noting that the manganese atoms exhibit larger magnetic moments than the iron ones and that the iron magnetic moment is markedly increasing when passing from antiferromagnetic to ferromagnetic state [5].

The refinement performed for the compositions with $y = 0.5$ and with $y = 0.3$ samples in the *ferromagnetic* states show that for the first sample the magnetic moments are found all directed along the c-axis, but for the second one the moments deviate from the c-axis by 50°. The easy axis direction is observed in the a–c plane.

In the case of the composition with $y = 0.275$, the refined data for the ferro states are different from the previous ones. All patterns, taken at three temperatures (1.45, 100, 135 K), show weak lines at small angles corresponding to the incommensurate state (Fig. 2). It should be noted that this content closely falls on the first order magnetoelastic transition boundary.

Finally, at the end of this paper it should be noted that the *short range* magnetic scattering is clearly visible for small Q-value range. It corresponds to the ferromagnetic correlations persisting well above the Curie or Néel point.

It remains in good agreement with previous magnetization study in high d.c. magnetic field [2, 4].

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