Magnetic Structure of $Mn_{0.95}Fe_{0.05}As$

KARI SELTE,[a] ARNE KJEKSHUS,[a] PER G. PETERZENS[a] and ARNE F. ANDRESEN[b]

[a] Kjemisk Institutt, Universitetet i Oslo, Blindern, Oslo 3, Norway and [b] Institutt for Atomenergi, Kjeller, Norway

As the first of a series of ternary arsenides ($T_{1-t}T'_tAs$; T,T' = V, Cr, Mn, Fe, Co) with MnP type structure we investigated $Mn_{1-t}Fe_tAs$.[1] After the data for other $Mn_{1-t}T_tAs$ phases [2,3] have become available, it has turned out that the variation in T_N (Néel temperature) with t for the double, a-axis helimagnetic mode characteristic of Mn-rich samples, appears to have a different trend for T = Fe than for T = V or Co. Since the T_N value for $Mn_{0.97}Fe_{0.03}As$ in Ref. 1 refers to a somewhat inhomogeneous sample with composition close to the phase boundary between the NiAs and MnP type structures, a new determination of T_N for a well defined sample, $Mn_{0.95}Fe_{0.05}As$, is reported here.

Experimental details concerning purity of elements, preparation of sample, neutron diffraction, and data reduction are as in Ref. 1.

The crystal structure of $Mn_{0.95}Fe_{0.05}As$ at and below room temperature is of the MnP type [1] and specified by the parameters given in Table 1.

The magnetic structure of $Mn_{0.95}Fe_{0.05}As$ is confirmed to be of the double, a-axis helical type with the following parameters at 95 K: $\mu_T = 1.45 \pm 0.05\ \mu_B$ (magnetic moment per metal atom), $\tau = (0.142 \pm 0.002) \times 2\pi\mathbf{a}^*$ (spiral propagation vector), $\phi = 72 \pm 5°$ (phase angle between independent spirals), and $\beta = 90°$ (angle between moment and spiral axis). With a value of 211 ± 1 K for T_N of $Mn_{0.95}Fe_{0.05}As$, the $Mn_{1-t}Fe_tAs$ phase fits nicely in with the other $Mn_{1-t}T_tAs$ phases. $Mn_{0.95}Fe_{0.05}As$ differs from $Mn_{0.90}Fe_{0.10}As$ [1] in that β is fixed at 90° in the former sample at all $T < T_N$, whereas β decreases from 90° at $T/T_N = 0.46$ to 60° at $T/T_N \approx 0.3$ in the latter. For the other parameters there is a resemblance between the two samples with respect to magnitude as well as their temperature variation (Fig. 1).

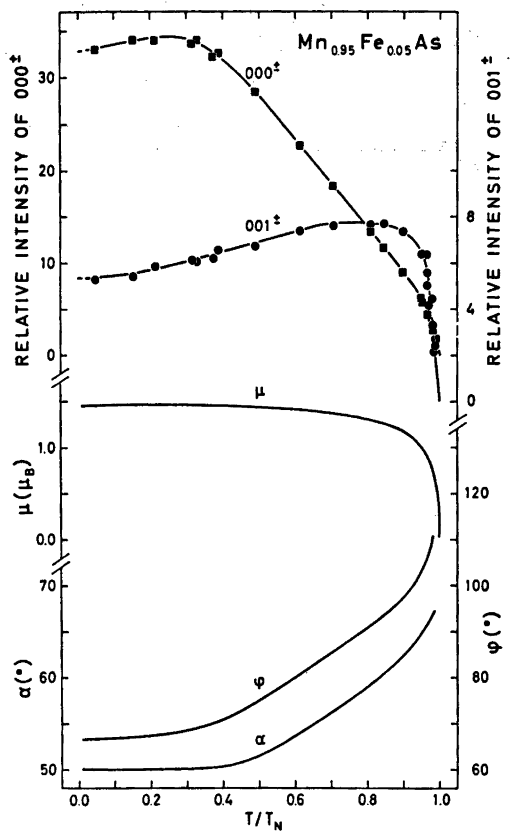

Fig. 1. Phase and turn angles and magnetic moments for spirals in $Mn_{0.95}Fe_{0.05}As$ together with relative intensities of satellite reflections 000± and 001± as functions of reduced temperature.

Table 1. Unit cell dimensions and positional parameters with standard deviations for $Mn_{0.95}Fe_{0.05}As$; space group *Pnma*, positions 4(*c*). (Overall profile reliability factors ranging between 0.033 and 0.046.)

T(K)	11	95	293
a(Å)	5.5384(5)	5.5574(6)	5.6425(4)
b(Å)	3.4863(3)	3.4995(4)	3.6008(4)
c(Å)	6.1472(7)	6.1686(9)	6.2858(8)
x_T	0.0063(21)	0.0056(19)	0.0088(17)
z_T	0.2036(17)	0.2058(20)	0.2120(15)
x_X	0.1971(7)	0.1982(8)	0.2118(6)
z_X	0.5796(8)	0.5804(9)	0.5797(10)

Indication of "doubled 000±" was also found for $Mn_{0.95}Fe_{0.05}As$, although much less pronounced than for $Mn_{0.90}Fe_{0.10}As$.[1] In the case of $Mn_{0.93}Fe_{0.05}As$, sample inhomogeneity is less probable and instrumental imperfections appear to provide the most likely explanation of the phenomenon.

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