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The Magnetic Structure of Tm_2Fe_{17}

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Recent magnetization and Mössbauer effect measurements (1) showed that in Tm_2Fe_{17} a change in the magnetic structure occurs at 72 K = T_o. At this temperature a pronounced maximum in the magnetization and an increase in the Fe hyperfine field are observed. It was suggested that this compound might exhibit a complex type of magnetic order between T_o and the Curie temperature T_c = 275 K. In the present note we report on the results of a neutron diffraction investigation of this compound.

The sample was prepared by arc melting of Tm, purity 99.9%, with Fe, purity 99.99%. Powder diagrams were recorded at the High Flux Reactor at Petten using λ = 2.57 Å and the usual 30' collimation. The angular range $0.012 < \sin\theta/\lambda < 0.362$ Å^{-1} was scanned at room temperature, 231, 80, and 4.2 K. In the subsequent analysis the scattering lengths were taken to be 0.720 and 0.951×10^{-12} cm for Tm and Fe, respectively. The Watson and Freeman (2) form factor for Fe^{2+} was used; the Tm^{3+} form factor was evaluated according to Blume et al. (3). For the refinements Rietveld's profile method (4) was applied.

At room temperature long range magnetic order was not observed. The crystal structure is known to be of the hexagonal Th_2Ni_{17} type, space group $P6_3/mmc$. Refinement of the structure parameters resulted in an R-factor based on intensities of 13%. It was possible to reduce the R-factor to 7% by allowing for disorder as proposed by Givord et al. (5) for Lu_2Fe_{17}. In doing so the composition $Tm_2Fe_{19.5}$ resulted, which does not agree with the homogeneity range of this compound, as determined by metallographic examination. However, we used the disordered model as a means of improving the values for the magnetic intensities at lower temperatures, taking advantage of the fact that nuclear and magnetic scattering are additive.

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Table 1

Position parameters for Tm_2Fe_{17} at 300 K, R = 13%.
Standard deviations in units of the last decimal are given in parenthesis

		x	y	z
Tm1	2(b)	0	0	1/4
Tm2	2(d)	1/3	2/3	3/4
Fe1	6(g)	1/2	0	0
Fe2	12(j)	0.323 (1)	-0.037 (1)	1/4
Fe3	12(k)	0.164 (1)	0.328 (2)	-0.013 (1)
Fe4	4(f)	1/3	2/3	0.109 (1)

Table 2

Cell constants as a function of temperature

T(K)	300	231	80	4.2
a(Å)	8.417 (1)	8.338 (6)	8.403 (1)	8.412 (1)
c(Å)	8.298 (1)	8.276 (7)	8.322 (1)	8.330 (1)
V($Å^3$)	509.1 (2)	498 (1)	509.7 (2)	510.7 (1)

Table 3

Magnetic moments in μ_B as a function of temperature

T (K)	300	231	80	4.2
μ(Tm)	-	0.0 (3)	4.2 (2)	6.4 (2)
μ(Fe)	-	-1.5 (3)	-2.2 (1)	-2.2 (1)

The structural parameters for the 13% refinement are given in Table 1. No temperature dependence was found. The cell constants are given in Table 2. Note that the thermal expansion coefficient is slightly negative in the ferrimagnetic region

Magnetic scattering was observed superimposed on the nuclear intensities at 231, 80, and 4.2 K. The magnetic structure was found to be collinear, the Tm and Fe sublattices being antiparallel. At 4.2 K the moments are along the c-axis; at 80 and 231 K they are in the ab plane. In Table 3 the magnitudes of the moments are given; it is seen that the Fe moment has reached its full value already at 80 K whereas the Tm moment rises only slowly to 6.4 μ_B/atom at 4.2 K, as compared to a free ion value of 7.6 μ_B.

At none of the temperatures considered evidence was found for a more complex type of magnetic order. The present results show that the difference in magnetization and hyperfine field above and below T_0 should be interpreted in terms of a change in magnetic anisotropy. Apparently the increase in hyperfine field at the Fe nucleus is not due to an increase in magnetic moment for Fe, but it may arise through an increase in the transferred field induced by the Tm moment.

Isostructural Y_2Fe_{17} and Y_2Co_{17} are known to have easy plane anisotropy (6). Recent model calculations (7) on R_2Co_{17} (R rare earth) compounds indicate that for Tm the preferred direction induced by the crystal field is parallel to the c-axis. The analysis is very likely applicable to Tm_2Fe_{17} as well. In going from higher temperatures, where the Tm moment is very low, to temperatures where the Tm moment is appreciable, one may expect a change from easy plane to easy axis anisotropy, in agreement with the present observation.

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