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THE ANTIFERROMAGNETIC STRUCTURE OF $TbMg_3$

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Depending on sample preparation, $TbMg_3$ undergoes ferromagnetic or antiferromagnetic ordering. The antiferromagnetic structure was determined by neutron diffraction. It consists of ferromagnetic (111) planes stacked along [111] antiferromagnetically. The moments are perpendicular to the (111) planes. Some order–disorder between Tb and Mg in the Fe_3Al-type structure and a slight excess (6 at.%) seems to be responsible for the observed antiferromagnetic structure.

1. Introduction

In a recent investigation [1] of the magnetic properties of RMg_3 compounds (R = rare earth) it was shown that the compounds with the light rare earths Ce, Pr and Nd undergo no magnetic order above 5 K. $SmMg_3$ orders antiferromagnetically at T_N = 6.5 K, while $GdMg_3$ and $TbMg_3$ indicated ferromagnetic behavior with ordering temperatures of 117 and 108 K, respectively. The magnetization measurements in the ferromagnetic compounds led to saturation moments which were only a fraction of the value $gJ\mu_B$. Also in $TbMg_3$ deviations from the Curie–Weiss behavior indicate a less perfect magnetic ordering. We have, therefore, studied $TbMg_3$ by neutron diffraction.

2. Experimental

For sample preparation we refer to refs. [1] and [2]. Two samples were prepared by different methods yielding different magnetic behavior. The one under investigation had an excess of 6 at.% Mg and showed antiferromagnetic behavior in its magnetization curves, with T_N = 20 K, θ_p = −110 K and a saturation moment of 9.56 μ_{eff}. The neutron diffraction experiments were done at the diffractometer KATINKA in the Kernforschungsanlage Jülich, on a powdered sample of 7 mm diameter. The wavelength was λ = 1.203 Å.

3. Neutron diffraction and magnetic structure

The diffraction diagrams obtained were rather poor, especially the magnetic peaks, with peak heights well below our commonly obtained intensities. X-ray diffraction experiments and Guinier film exposures were done in order to check the crystallinity, and again rather broad peaks in the order of 0.65° in 2 θ were recorded. Annealing or heating of the sample did not improve the diagrams; heating above 600°C led to decomposition of the sample.

$TbMg_3$ crystallizes with the cubic Fe_3Al-type structure, space group O_h^5-Fm3m with Tb in *a*: 000, Mg(1) in 8 *c*: $\frac{1}{4}\frac{1}{4}\frac{1}{4}$; $\frac{3}{4}\frac{3}{4}\frac{3}{4}$ and Mg(2) in 4 *b*: $\frac{1}{2}\frac{1}{2}\frac{1}{2}$. The Fe_3Al-type structure is related to the CsCl-type structure by an ordered replacement of every other atom at 000 in the CsCl-structure. The observed diffraction diagrams indicate that in the sample under investigation this order is not perfect, and there is some degree of disorder in the Tb–Mg distribution.

The neutron diffraction diagram recorded at 5 K

Table 1
Comparison between observed ($I_o^{mag.}$) and calculated ($I_c^{mag.}$) intensities of magnetic reflections at 4.2 K

2θ	h	k	l	$I_o^{mag.}$	$I_c^{mag.}$
15:72	3	1	1	7038	6995
20.70	1	3	3	1860	2110
24.74	1	5	1	880	937
28.23	5	3	1	3100	2990
31.37	5	3	3	1250	1176
34.24	5	1	5	750	904
	1	7	1		

clearly reveals additional superlattice peaks, which can be indexed on the basis of a doubled cubic unit cell $a_M = 2a_0$ in all three directions. Table 1 lists the magnetic reflections with observed and calculated intensities. The diagram resembles antiferromagnetic MnO except for the absence of the 111 (and 333) reflection. The magnetic structure (fig. 1) consists of ferromagnetic (111) planes stacked along [111] in antiparallel sequence.

In cubic symmetry the direction of the moments cannot be determined; the magnetic interaction vector q has a mean value of $|q|^2 = \frac{2}{3}$ for all allowed peaks. The absence of the 111-peak requires, therefore, rhombohedral symmetry at least of the magnetic lattice and, via the magnetic interaction vector q ($q^2 = \sin^2\alpha$), the direction of the moment vector μ is determined as being perpendicular to the (111) planes (along [111]).

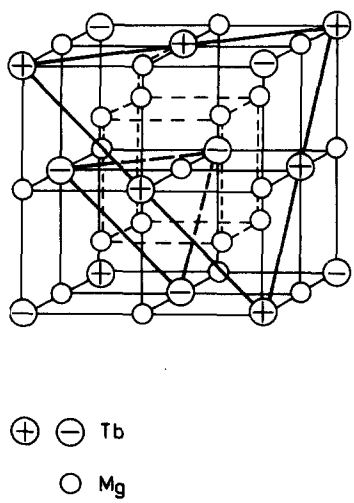

Fig. 1. Crystal structure (Fe_3Al-type) and ordered magnetic structure of $TbMg_3$. The moments are perpendicular to the indicated (111) planes.

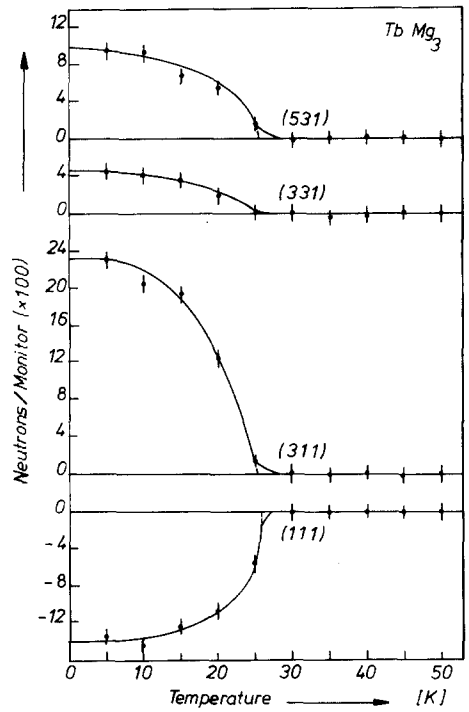

Fig. 2. Temperature dependence of four antiferromagnetic peaks yielding a Néel-temperature of $T_N = 26$ K.

The observed and calculated intensities corraborate this model. Full evaluation of the data leads to a moment of 9.59 μ_{eff}. We trace this discrepancy to some disorder in the Tb distribution, and also to some extent to crystal field effects.

In fig. 2 the temperature dependence of four magnetic peaks is depicted, yielding a Néel temperature of $T_N = 26 \pm 1$ K. This discrepancy to $T_N = 21$ K from magnetization measurements is not quite clear and may be due to differences in the samples used for magnetization measurements and neutron diffraction.

4. Discussion

Molecular field calculations [2] show that in both compounds $GdMg_3$ and $TbMg_3$, ferromagnetic and antiferromagnetic interactions are in the same order of magnitude. Slight changes in the composition or in the Tb–Mg order–disorder parameters will therefore

shift this ratio of interactions significantly and can, therefore, also affect the magnetic structure and the transition temperature.

Acknowledgement

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References

[1] K.H.J. Buschow, J. Less Common Metals 44 (1976) 301.
[2] K.H.J. Buschow, G. Will and M.O. Bargouth (in preparation).