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Neutron diffraction studies of $TbMn_2D_x$ and $ErMn_2D_2$

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Abstract

The results of neutron diffraction investigations on $TbMn_2D_2$, $TbMn_2D_3$ and $ErMn_2D_2$ are presented and analysed. The magnetic ordering temperatures of $TbMn_2D_x$ are 284 and 299 K for $x = 2$ and 3, respectively. Their magnetic structures are antiferromagnetic and collinear with the propagation vector $[\frac{1}{2},\frac{1}{2},\frac{1}{2}]$. The $ErMn_2D_2$ orders magnetically at about 214 K. The differentiated temperature behaviour of Mn and rare earth (Tb and Er) magnetic sublattices is observed. The magnetic moments of Mn and rare earths have different temperature dependence.

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Keywords: Neutron diffraction; Metal hydrides; Magnetic structures

1. Introduction and experimental details

In our research we focused on the influence of hydrogen (deuterium) on the magnetic structure in $REMn_2$ compounds (RE = rare earth). On the basis of the structural and magnetic investigations of the series $TbMn_2H_x$ [1] and $ErMn_2H_x$ [2] the deuterides remaining as single phase in the whole temperature range: $TbMn_2D_2$, $TbMn_2D_3$, and $ErMn_2D_2$ were chosen for the neutron diffraction studies. In our report on neutron diffraction in $TbMn_2D_2$ [3] we concluded, that the system orders antiferromagnetically with a propagation vector $\mathbf{k} = [\frac{1}{2},\frac{1}{2},\frac{1}{2}]$. The powdered deuterides were made using the standard technique [1]. The neutron diffraction measurements were made at ILL Grenoble.

2. Results and interpretation

To complete the data for $TbMn_2D_2$ we made the temperature scan which allowed to determine the ordering temperature $T_N = 284$ K (Table 1). The magnetic transition is of first-order type and is associated to the strong antiferromagnetic Mn–Mn exchange interactions. This is visible in almost temperature independent behaviour of magnetic lines (Fig. 1). However some magnetic lines corresponding to the Tb ordering contribution exhibit a strong temperature dependence.

Weakly coupled Tb 4f type moments can strongly fluctuate at higher temperatures close to T_N, so their contribution to diffraction lines increases when lowering the temperature.

The neutron diffraction spectra for $TbMn_2D_3$ obtained between 2 and 320 K are similar to those obtained on $TbMn_2D_2$. At room temperature the deuterium atoms are distributed randomly also at the 96g site. The compound orders antiferriomagnetically below $T_N = 299$ K with the same propagation vector $\mathbf{k} = [\frac{1}{2},\frac{1}{2},\frac{1}{2}]$ as for $TbMn_2D_2$, with the Tb moment (4.4 μ_B), the manganese moments Mn1 (4.3 μ_B) and Mn2–4 (2.4 μ_B).

The value of Tb moment is comparable with that in $TbMn_2D_2$ and values of Mn2–4 moments are about two times increased reaching the values comparable with those in $TbMn_2D_{4.5}$ [4] which is reflected by increase of Mn–Mn distances. The reduced value of Tb magnetic

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Table 1

Deuteride	Structure	T_N (K)	Magnetic structure
$TbMn_2D_2$	Fd3m (4–300 K)	284 (±5)	AF collinear
$TbMn_2D_3$	Fd3m (4–300 K)	299 (±8)	AF collinear
$ErMn_2D_2$	$P6_3/mmc$ (250 K)	214 (±8)	AF non-collinear?
	P1 (4 K)		
	Deuterium position (at 250 K):		
	D1 (0.057; 0.312; 0.573), D2 (0.455; 0.911; 0.640)		
	D3 (0.492; 0.961; 0.250), D4 (0.135; 0.270; 0.250)		

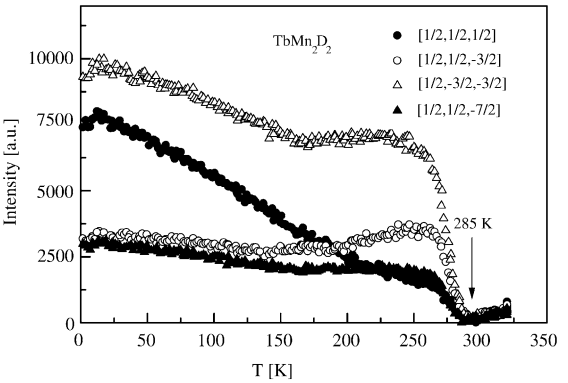

Fig. 1. Temperature dependencies of the magnetic lines in the diffraction patterns for $TbMn_2D_2$.

moment can be caused by crystal field interactions. The temperature dependencies of magnetic peaks are also similar to those observed for $TbMn_2D_2$.

The most complicated situation is for the hexagonal $ErMn_2D_2$. The high temperature patterns (250 K) is characteristic of nuclear hexagonal ($P6_3/mmc$) C14 structure.

The deuterium atoms are distributed on four crystallographic sites namely: 24l, 12k and two 6h. From the temperature scan the magnetic ordering temperature $T_N = 214$ K was obtained. However, the diffraction pattern for the magnetically ordered state is very complex. The low temperature patterns show, in addition to the nuclear peaks, many peaks of magnetic origin (Fig. 2). No contribution to the intensity of the nuclear peaks was observed excluding either ferromagnetic contribution nor antiferromagnetic with $k = 0$ propagation vector. Some of these peaks could be explained assuming propagation vector $\mathbf{k} = [\frac{1}{4}, \frac{1}{4}, 0]$. In addition, the low temperature pattern is complicated by

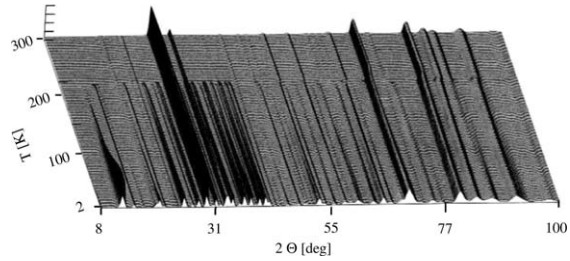

Fig. 2. $ErMn_2D_2$—temperature patterns.

the triclinic structure distortion below 214 K [2] as it confirmed by the X-ray diffraction.

The intensity of some of the extra lines in the diffraction patterns increase strongly at lowering temperature showing the magnetic ordering of the Er sublattice and its strong magnetic dependence.

Acknowledgements

The work is in progress to solve completely the magnetic structure in $ErMn_2D_2$.

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