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MAGNETIC ORDERING IN $NdRh_2Si_2$ AND $ErRH_2Si_2$

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Neutron diffraction and magnetization study of polycrystalline $NdRh_2Si_2$ and $ErRh_2Si_2$ was performed in the temperature range from 4.2 to 293 K. Both compounds are of $ThCr_2Si_2$ type crystal structure and exhibit antiferromagnetic ordering below $T_N = 53$ K and $T_N = 12.8$ K respectively. The magnetic structure wave vector is $\tau = [0, 0, 1]$.

1. INTRODUCTION

MAGNETIC PROPERTIES of $RERh_2Si_2$ intermetallics attracted lately considerable attention. Felner and Novik [1] claim that all $RERh_2Si_2$ compounds are antiferromagnetic at low temperatures, Ślaski *et al.* [2] in a recent paper have shown by neutron diffraction that $TbRh_2Si_2$ and $HoRh_2Si_2$ are collinear antiferromagnets with wave vector $\tau = [0, 0. 1]$, while Quezel *et al.* report that $CeRh_2Si_2$ exhibit collinear antiferromagnetic ordering with wave vector $\tau = [\frac{1}{2}, \frac{1}{2}, 0]$ [3]. We have included into our programme two other members of $RERh_2Si_2$ series, i.e. $NdRh_2Si_2$ and $ErRh_2Si_2$ and present the results of neutron diffraction and magnetization measurements in this note.

2. EXPERIMENT AND RESULTS

The samples were synthetized by direct melting of elements in an arc furnace under purified argon atmosphere. X-ray diffraction tests show that both samples are single phases with $ThCr_2Si_2$ type structure and lattice parameters listed in Table 1. They are in good agreement with those ones reported previously [1].

Magnetometric measurements were carried out in the temperature range between 4.2 and 300 K using a vibrating sample magnetometer of Foner type. In addition, magnetization curves were obtained at 4.2 K in external magnetic fields up to 5 T. The results of magnetometric measurements are presented in Figs. 1 and 2.

Table 1. Crystal structure parameters of $NdRh_2Si_2$ *and* $ErRh_2Si_2$

Compound	a (10^{-1} nm)	c (10^{-1} nm)	c/a	V (10^{-1} nm)^3	z	R (%)	Ref.
$NdRh_2Si_2$	4.059(3)	10.003(5)	2.464	164.80(33)	0.3725(8)	5.96	*
	4.069(2)	10.11(1)	2.485	167.39(33)	–	–	[1]
$ErRh_2Si_2$	4.025(3)	9.958(8)	2.474	161.33(34)	0.3764(12)	7.1	*
	4.012(2)	9.88(1)	2.463	159.03(32)	–	–	[1]

* This study.

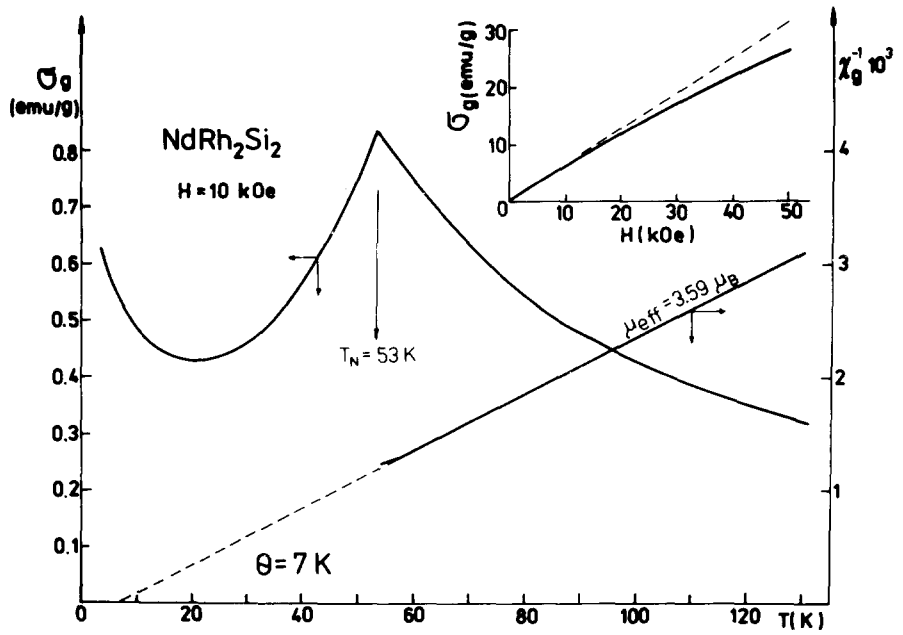

Fig. 1. Temperature dependence of magnetization and reciprocal magnetic susceptibility of $NdRh_2Si_2$. The inset shows magnetization curve at 4.2 K.

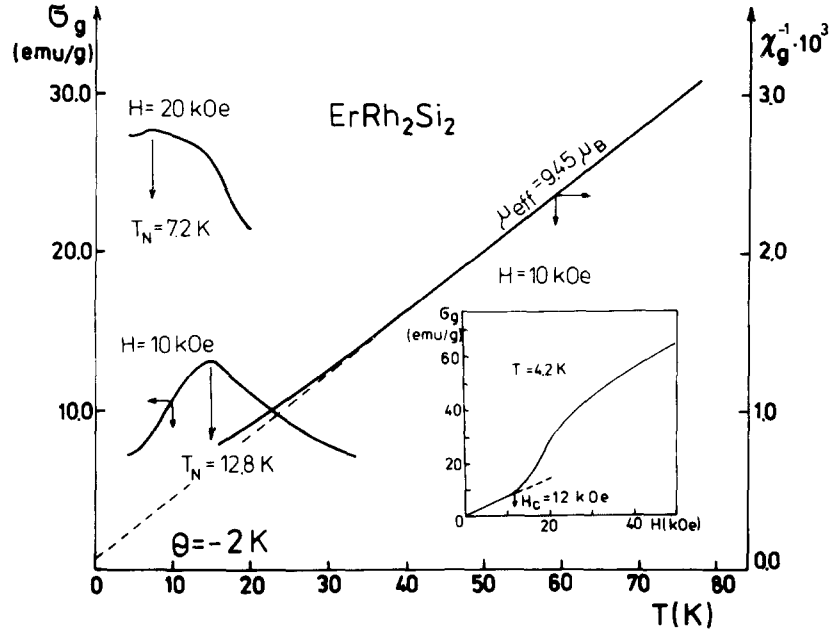

Fig. 2. Magnetization and reciprocal susceptibility versus temperature curves for $ErRh_2Si_2$. Magnetization curve at 4.2 K is displayed in the inset.

$NdRh_2Si_2$ orders antiferromagnetically at $T_N = 53$ K. The magnetic susceptibility follows the Curie–Weiss law. The effective moment value $\mu_{eff} = 3.59\,\mu_B$ is in fair agreement with that one of a free ion of neodymium in trivalent state. The paramagnetic Curie temperature is positive: $\theta_p = 7$ K. The above data differ significantly from those ones published by Felner and Novik [1], i.e. $\theta_p = -4$ K, $\mu_{eff} = 4.7 \pm 0.1\,\mu_B$.

$ErRh_2Si_2$ orders also antiferromagnetically at 4.2 K. Magnetic susceptibility obeys the Curie–Weiss law above $T_N = 12.8$ K. The paramagnetic Curie temperature is $\theta_p = -2$ K. The measured effective moment of $9.45\,\mu_B$

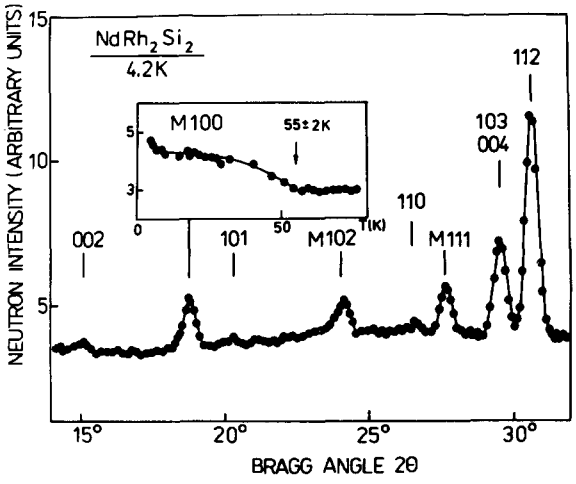

Fig. 3. A part of neutron diffractogram of $NdRh_2Si_2$ obtained at 4.2 K.

is close to the Er^{3+} free ion value ($9.59\,\mu_B$). Magnetization isotherm for $ErRh_2Si_2$ is linear up to 1.25 T. At this value a phase transition is observed. Neutron diffraction data ($\lambda = 1.326 \times 10^{-1}$ nm) were collected by means of the DN-500 diffractometer at the EWA reactor in Świerk. Neutron diffraction patterns were taken at 293 K (RT) and 4.2 K) (LHT), while the temperature dependence of magnetic peak intensities was measured for the temperature range 4.2–80 K. The observed neutron intensities were treated with the Rietveld line profile analysis method. Nuclear scattering lengths $b_{Er} = 0.79, b_{Nd} = 0.72, b_{Rh} = 0.59, b_{Si} = 0.415 \times 10^{-14}$ m were used. The magnetic form factor Nd^{3+} and Er^{3+} were taken from [4, 5].

Room temperature diffractograms of the above two compounds consist of strong reflections, satisfying the condition $h + k + l = 2n$. Nuclear intensities were calculated for the RE atoms in positions 2(*a*), Rh in 4(*d*) and Si in 4(*e*) of the space group $I4/mmm$. The best fit was achieved for the parameters given in Table 1.

In the neutron diffraction diagram of $NdRh_2Si_2$ displayed in Fig. 3 additional reflections can be identified at $T = 4.2$ K. They are indexable on the same unit-cell as the crystallographic one, however with the indices obeying $h + k + l = 2n + 1$ rule. An antiferromagnetic ordering of the same kind as observed previously in $RECo_2Si_2$ [5–7] and $TbRh_2Si_2$ [2] can be thus deduced. It is usually called $+-+-$ type since it can be visualized as sequences of ferromagnetic sheets coupled antiferromagnetically along the *c*-axis. The absence of the 001, 003 magnetic peaks indicates without any ambiguity that the moments are aligned along the *c*-axis. A moment value $\mu = 3.25 \pm 0.15\,\mu_B$ at $T = 4.2$ K indicates that the nedymium magnetic moment is equal to the free ion value ($g_J J = 3.27\,\mu_B$). There is no evidence of any magnetic moment on the rhodium atoms.

The temperature dependence of the M100 magnetic peak intensity shown in inset in Fig. 3 gives the ordering temperature $T_N = 55$ K.

Neutron diffraction diagrams given in Fig. 4 show that $ErRh_2Si_2$ develops at low temperatures, a magnetic order different from that found in $NdRh_2Si_2$. The presence of magnetic reflections M001 and M003 indicates that magnetic moment on Er forms an angle ϕ with the tetragonal axis. From the analysis of peak intensities it follows that ϕ amounts to 90°. $ErRh_2Si_2$ is thus an antiferromagnet with Er magnetic moments in the basal plane. The coupling within this plane is ferromagnetic, but antiferromagnetic between adjacent

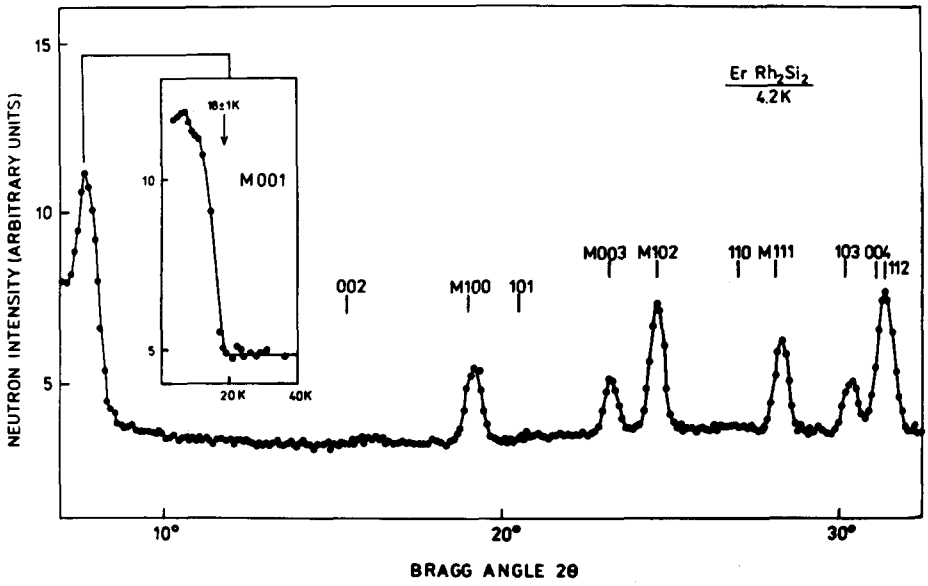

Fig. 4. A part of LHT neutron diffraction pattern of $ErRh_2Si_2$.

Table 2. Magnetic data for $NdRh_2Si_2$ *and* $ErRh_2Si_2$

Compound	T_N (K)		θ_p (K)	Magnetic moment (μ_B)				Ref.
	M	*ND*		μ_{eff}	$g\sqrt{J(J+1)}$	μ	gJ	
$NdRh_2Si_2$	53	55 ± 1	7	3.59	3.58	3.25(15)	3.27	*
	56	–	−4	4.7		–		[1]
$ErRh_2Si_2$	12.8	18 ± 1	−2	9.45	9.59	7.74(27)	9.0	*
	13	–	8	7.6		–		[1]

* This study.

planes. A moment value $\mu = 7.74 \pm 0.27\,\mu_B$ is found at $T = 4.2$ K indicating that the erbium magnetic moment is close to the free ion value.

The Néel point was determined with rather poor accuracy to be (18 ± 1) K. Other magnetic data are listed in Table 2.

3. CONCLUSIONS

1. Our neutron diffraction data indicate that only Nd and Er ions carry localized magnetic moment. It amounts close to the free ion value of Nd^{3+} and Er^{3+} (Table 2). No localized moment on Rh atom is observed within the accuracy of the experiment.

2. A magnetic phase transition in $ErRh_2Si_2$ at 4.2 K in magnetic field of 1.25 T takes place. Antiferromagnetic order transforms into ferromagnetic one.

3. $NdRh_2Si_2$, $TbRh_2Si_2$ (2), $HoRh_2Si_2$ (2) and $ErRh_2Si_2$ exhibit a simple collinear antiferromagnetic structure with propagation vector $\tau = [0, 0, 1]$, however, a change in moment alignment occurs passing from Tb to Er compound. In $NdRh_2Si_2$ and $TbRh_2Si_2$ the magnetic moment is along the *c*-axis, in $HoRh_2Si_2$ it forms the angle $\phi = (28 \pm 3)^\circ$, while in $ErRh_2Si_2$ it is normal to the *c*-axis. We have observed earlier the same regularity in $RECo_2Si_2$ compounds [6, 7] which are magnetically isostructural with $RERh_2Si_2$: neutron diffraction study of $ErCo_2Si_2$ shows that moment is normal to the *c*-axis while in other members of this family it is along the *c*-axis. The orientation of magnetic moment in respect to the crystallographic unique axis is connected with the sign of B_2^0 coefficients in CEF Hamiltonian. According to Greedan and Rao [8] the positive sign of B_2^0 implies that the moment lies in the basal plane or makes an angle ϕ with the *c*-axis. The change of sign occurs usually when passing from Ho to Er in the RE series [9] resulting in different orientation of magnetic moment in Er and Tm compounds, in agreement with the results of neutron diffraction and Mössbauer experiments.

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