Journal of Magnetism and Magnetic Materials 30 (1983) 355–358
North-Holland Publishing Company

THE ANTIFERROMAGNETIC STRUCTURE OF $ErCo_2Si_2$ BY NEUTRON DIFFRACTION

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Received 18 June 1982; in revised form 23 August 1982

The magnetic structure of the tetragonal $ErCo_2Si_2$ compound is determined by neutron diffraction on powder sample at 4.2 K. The magnetic ordering is connected with a symmetry lowering, magnetic space group $P_{2_s}\bar{1}$ $(Sh_2^7)k = 000$. The structure is collinear antiferromagnetic with the erbium magnetic moments making an angle of 56.2° with the c axis. The magnetic moment value for erbium is $6.75\mu_B$.

1. Introduction

The crystal structures of the RT_2Si_2 compounds, where R is a rare earth metal and T a transition metal have been extensively studied [1–4]. Susceptibility measurements on RT_2Si_2 show that the majority of these compounds are antiferromagnetic [5–7]. Our purpose is to reveal the magnetic structures of these compounds starting in the present study with $ErCo_2Si_2$ of the RCo_2Si_2 series.

The $ErCo_2Si_2$ compound crystallizes in the tetragonal $ThCu_2Si_2$ type-structure with the space group I4/mmm (D_{4h}^{17}) [4]. The erbium, cobalt and silicon atoms occupy in the unit cell the 2(a), 4(d) and 4(e) sites, respectively. Magnetic measurements on $ErCo_2Si_2$ show that this compound orders antiferromagnetically with Néel temperature equal to 6 K [7].

2. Experimental

The sample was prepared from 99.9% pure Er and 99.9% pure Co and Si by melting the starting materials in a high frequency induction furnance under purified argon atmosphere and was remelted several times. X-ray powder diffraction showed that the sample is single phase. The lattice parameters were found to be in fair agreement with those determined by Rossi et al. [4].

The neutron diffraction powder data were recorded with the two-axis spectrometer at the reactor Saphir, Würenlingen (= 2.339 Å) at the temperatures 293 and 4.2 K. The observed neutron intensities were corrected for absorption and evaluated by the line profile analysis method [8].

3. Results

3.1. The nuclear structure at 293 K

The neutron diffraction diagram at 293 K shows the systematic absence of the hkl reflections with $h + k + l = 2n + 1$. As expected all nuclear lines could be indexed with the tetragonal body-centered lattice which is double primitive. The refinement of the nuclear intensities was carried for various sets of parameters. The used nuclear scattering lengths are $b_{Er} = 0.79$, $b_{Co} = 0.25$ and $b_{Si} = 0.42 \times 10^{-12}$ cm [9]. The best fit was achieved for the parameters given in table 1. The use of individual temperature factors did not improve the refine-

0304-8853/83/0000–0000/$03.00

Table 1
Refined parameters from neutron intensities of $ErCo_2Si_2$ at 293 and 4.2 K. The estimated standard deviations are in parenthesis and correspond to the last digits. R_n, R_m and R_{wp} are the agreement values for nuclear, magnetic and weighthed profile intensities [8]. The atomic position of silicon is 0.0; 0.0; z_{Si}. B_{OTF} is the overall temperature factor

T (K)	R_n	R_{wp}	R_m	a (Å)	c (Å)	z_{Si}	B_{OTF} (Å^2)
293	0.13	0.16	–	3.8758(8)	9.7275(28)	0.37472(65)	0.5
4.2	0.13	0.15	0.06	3.8599(5)	9.7097(24)	0.3757(10)	0.5

$\mu_{Er}(\mu_B) = 6.746(79)$, $\varphi = 56°.2$.

ment. Several attempts of refinement using the possible subgroups of first generation (with the same translation) of the I4/mmm space group remained also unsuccessful. A further symmetry lowering on the basis of the present powder data results to an unfavourable relation of parameters to observation. Most likely the rather poor reliability factor for the nuclear intensities may be connected with preferential orientation effects or overlapping impurity lines. Fig. 1 displays the calculated and observed profiels at 293 K.

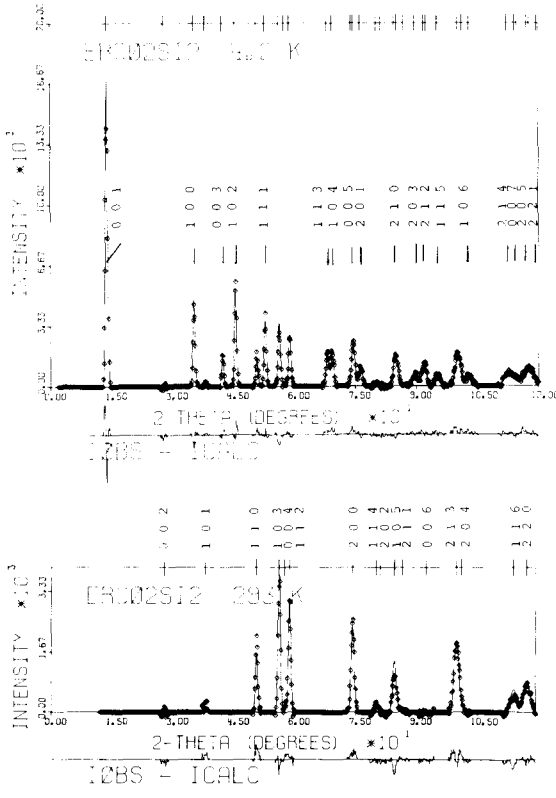

Fig. 1. Neutron diffraction patterns from paramagnetic (293 K) and ordered (4.2 K) $ErCo_2Si_2$. The full curve is the calculated profile and the points are the observed intensities. The difference diagram is below. For clarity only the magnetic lines are indexed at 4.2·K $h + k + l = 2n + 1$.

3.2. Magnetic structure at 4.2 K

In the 4.2 K neutron diffraction diagram besides the nuclear peaks indexed in the body-centered tetragonal lattice (hkl with $h + k + l = 2n$) new superlattice lines of magnetic nature ap-

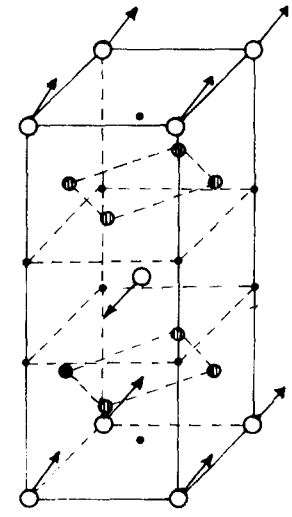

Fig. 2. The magnetic structue at 4.2 K of $ErCo_2Si_2$ (○ Er, ◍ Co, • Si).

Table 2
Calculated and observed neutron intensities of $ErCo_2Si_2$ including the powder multiplicity and Lorentz factor, at 4.2 K

hkl	$I_{nuc.}$	$I_{mag.}$	$I_{tot.}$	$I_{obs.}$	*hkl*	$I_{nuc.}$	$I_{mag.}$	$I_{tot.}$	$I_{obs.}$
001	–	75054	75054	76288	202	493	–	493	0
002	754	–	754	0	105	10384	–	10384	9548
100	–	20746	20746	19644	210	–	6384	6384	6234
101	709	–	709	1269	211	388	–	388	276
003	–	7430	7430	8032	203	–	5888	5888	6745
102	–	24606	24606	25780	212	–	11180	11180	12065
110	7225	–	7225	8334	006	88	–	88	73
111	–	17558	17558	17335	115	–	5410	5410	6924
103	18002	–	18002	15501	213	17478	–	17478	21447
004	463	–	463	511	204	929	–	929	1240
112	14857	–	14857	14823	106	–	4828	4828	6241
113	–	10329	10329	12451	214	–	8465	8465	8975
104	–	10116	10116	12188	116	7166	–	7166	6881
005	–	2237	2237	2917	007	–	1074	1074	1159
200	14098	–	14098	16071	205	–	4118	4118	4995
201	–	7991	7991	7663	220	10174	–	10174	11285
114	1712	–	1712	848	221	–	3962	3962	3602

pear. All magnetic peaks can be indexed using the same cell as the chemical one but not with the same body centered tetragonal lattice, which is double primitive.

The magnetic lattice is primitive and the magnetic reflections *hkl* obey the limiting condition: $h + k + l = 2n + 1$. This suggests that the non-primitive lattice translation (1/2 1/2 1/2) has become an antitranslation. Compared to the primitive tetragonal cell the magnetic cell is doubled in three directions with the magnetic wave vector $k = 1/2\ 1/2\ 1/2$. On the other hand, if we refer to the body centered chemical cell, the magnetic wave vector is $k = 000$, but the magnetic lattice is primitive I_p.

The collinear antiferromagnetic model used to refine the magnetic structure assumes that the Er atoms at the lattice positions 000 and 1/2 1/2 1/2 have their moments opposite. This model explains the 4.2 K neutron data satisfactorily (tables 1 and 2, fig. 1 and 2). The resulting magnetic moment of erbium is $6.75\mu_B$ and makes an angle of 56.2° with the *c* axis of the crystal fig. 2. All refined parameters are summarized in table 1. The magnetic form factor Er^{3+} was taken from ref. [10].

The existence of a moment component perpendicular to the fourfold axis results to a symmetry lowering of the magnetic structure. The corresponding magnetic space group is $P_{2_s}\bar{1}$ (Sh_2^7).

Most probably the ordered moment value of erbium $6.75\mu_B$ at 4.2 K is well below the saturation value of the free ion Er^{3+} ($gJ = 9\mu_B$) because of the low ordering temperature $T_N = 6$ K. Cobalt seems to carry no magnetic moment, this may be due to the total filling of the cobalt 3d-band by conduction electrons. Silicon is non-magnetic.

Acknowledgement

We would like to express our gratitude to Prof. Dr. W. Hälg, ETHZ, Institut für Reaktortechnik, for the support of this work.

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