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THE MAGNETIC STRUCTURE OF $HoCo_2Si_2$

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Abstract—We have carried out neutron diffraction on a $HoCo_2Si_2$ powder sample at 4.2 K. The magnetic structure of this compound is collinear antiferromagnetic with the holmium magnetic moments parallel to the c-axis of the crystal. The magnetic moment value of holmium is 9.85 μ_B. The magnetic space group is $I4/mm'm'$ (Sh^{410}_{128}) $k = 000$. The ordering temperature is $T_N = 12(1)$ K.

INTRODUCTION

The compound $HoCo_2Si_2$ crystallizes in the tetragonal $ThCu_2Si_2$ type-structure with the space group $I4/mmm$ (D^{17}_{4h}) [1]. The holmium, cobalt and silicon atoms occupy in the unit cell the 2(a), 4(d) and 4(e) sites respectively. Previous magnetic susceptibility measurements on $HoCo_2Si_2$[2] show an ordering temperature of 15 K, and a negative paramagnetic Curie-temperature of −8 K (indicating antiferromagnetism).

In the present study we report a model for the magnetic structure of $HoCo_2Si_2$, derived from neutron diffraction powder data at 4.2 K. In addition we describe the temperature dependance of the magnetic intensity and magnetic moment.

EXPERIMENTAL

The sample was prepared 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 agreement with those determined by Rossi *et al.*[1].

The neutron diffraction powder data were recorded with the two axis spectrometer at the reactor Saphir, Würenlingen ($\lambda = 2.343$ Å) at the temperatures 293 and 4.2 K. The step increment in 2θ used for the data was 0.15 deg. The observed neutron intensities were corrected for absorption and evaluated by the line profile analysis method[3].

The nuclear structure at 293 *K*

The neutron diffraction diagram at 293 K shows the systematic extinction of the hkl reflections with $h + k + l = 2n + 1$.

All nuclear lines have been indexed with the tetragonal body-centered lattice. The nuclear scattering lengths used are $b_{Ho} = 0.85$, $b_{Co} = 0.25$, and $b_{Si} = 0.42 \times 10^{-12}$ cm[4].

The best fit was achieved for the parameters given in Table 1. The reliability factor for the nuclear intensities is 8%. Fig. 1 displays the calculated and observed profiles at 293 K.

The 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 appear. The magnetic cell has the same size as the nuclear one, but the magnetic lattice is primitive similar to $ErCo_2Si_2$[5]. All magnetic lines follow the rule $h + k + l = 2n + 1$, characteristic for the $\frac{111}{222}$ antitranslation operation. On the other hand from the zero intensity of the 001 magnetic line it can be assumed

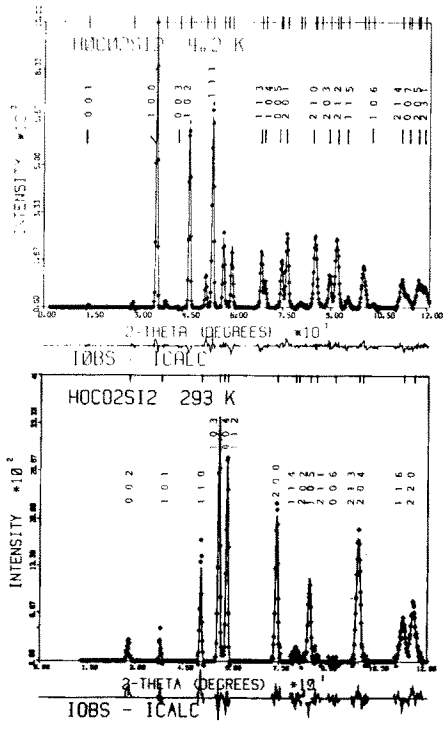

Fig. 1. Neutron diffraction patterns from paramagnetic (293 K) and ordered (4.2 K) $HoCo_2Si_2$. The full curve is the calculated profile and the points are the observed intensities. The difference diagram is below. For clarity only the magnetic lines are indexed at 4.2 K $h + k + l = 2n + l$.

Table 1. Refined parameters from neutron intensities of $HoCo_2Si_2$ at 293 and 4.2 K. R_n, R_m, R_{wp} are the agreement values for nuclear, magnetic and weighted profile intensities. R_{exp} is the expected agreement value depending on the statistical accuracy of the data[3]. B_{OTF} = Overall temperature factor

T[K]	R_n	R_m	R_{wp}	R_{exp}	a(Å)	c(Å)	z_{Si}	B_{OTF}(Å^2)
293	8%	-	16%	7%	3.8799(9)	9.735(2)	0.3734(6)	0.7(1)
4.2	8%	4%	10%	5%	3.8718(3)	9.731(1)	0.3763(7)	0.23(8)

μ_{Ho} = 9.856(73) μ_B

Table 2. Calculated and observed neutron intensities of $HoCo_2Si_2$ including the powder multiplicity and Lorentz factor, at 4.2 K

hkl	$I_{nucl.}$	$I_{mag.}$	$I_{tot.}$	$I_{obs.}$	hkl	$I_{nucl.}$	$I_{mag.}$	$I_{tot.}$	$I_{obs.}$
001	-	128	128	213	202	348	-	348	744
002	512	-	512	431	105	7399	-	7399	7591
100	-	42136	42136	42789	210	-	12922	12922	13281
101	81-	-	814	1062	211	462	-	462	867
003	-	13	13	0	203	-	8673	8673	9154
102	-	29882	29882	28766	212	-	19997	19997	20643
110	4553	-	4553	5764	006	53	-	53	48
111	-	32832	32832	32860	115	-	3558	3558	2786
103	12278	-	12278	12557	213	12356	-	12356	12838
004	488	-	488	586	204	1015	-	1015	719
112	11371	-	11371	10204	106	-	1404	1404	786
113	-	11900	11900	10991	214	-	11223	11223	10398
104	-	5562	5562	5595	116	5565	-	5565	4454
005	-	4	4	110	007	-	2	2	1
200	10047	-	10047	10587	205	-	4101	4101	3867
201	-	15483	15483	17257	220	7498	-	7498	7419
114	1040	-	1040	1197	221	-	7895	7895	8332

that there is no moment component in the *xy* plane in contrast to $ErCo_2Si_2$.

The collinear antiferromagnetic model used to refine the magnetic structure assumes that the holmium atoms at 000 and 1/21/21/2 have their moments opposite. The refinement resulted in a moment direction parallel to the *c* axis. The corresponding magnetic space group is tetragonal and primitive I_P $4/mm'm'$[6] or P_I $4/mnc$ (Sh^{410}_{128})[7], in contrast to the $ErCo_2Si_2$ (monoclinic).

The magnetic form factor used for Ho^{3+} is that of Ref. [8]. The refined magnetic moment of holmium is found to be 9.85 μ_B. This model, Fig. 2 explains the 4.2 K neutron data satisfactory (Tables 1 and 2, Fig. 1) as well as the theoretical form factor curve of Ref. [8], Fig. 3.

All refined parameters are summarized in Table 1. The reliability factor for the magnetic intensities is 4%. The ordered moment value of holmium at 4.2 K (9.85 μ_B) is close to the saturation value ($g_J J$ = 10 μ_B) of the free ion Ho^{3+}. Silicon is non magnetic. Cobalt seems to carry no magnetic moment, probably because of the total filling of its 3*d*-band by conduction electrons.

Temperature dependence measurements

According to the magnetic data reported in [2] $HoCo_2Si_2$ orders ferromagnetically at 15 K. The 4.2 K neutron data demonstrate that the compound is a collinear antiferromagnet. In order to understand the discrepancy between the results of the two methods a temperature dependence measurement was undertaken. No phase transition to a ferromagnetic structure could be detected over the temperature range 4.2–15 K. We

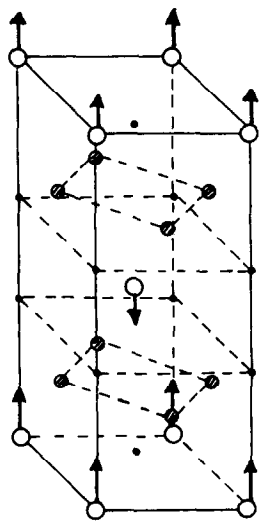

Fig. 2. The magnetic structure at 4.2 K of $HoCo_2Si_2$ (○ Ho, ⊘ Co, • Si).

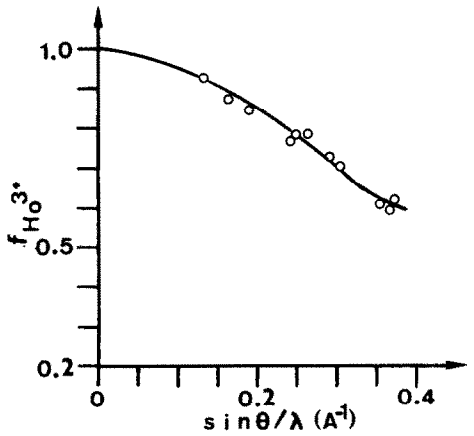

Fig. 3. The sin θ/λ dependance of the Ho^{3+} magnetic form factor. The circles are the experimental values and the full curve the theoretical values [8].

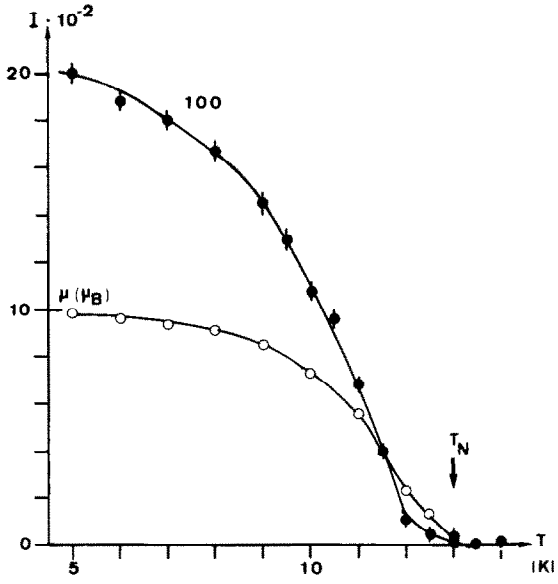

Fig. 4. Temperature dependance, a) of the magnetic intensity of the 100 peak (full circles), b) of the ordered magnetic moment of Ho^{3+} (open circles).

therefore assume that $HoCo_2Si_2$ is antiferromagnetic up to the paramagnetic transition at 15 K. Most likely the discrepancy is related to the difficulty in finding the minimum on the rather flat susceptibility curve [2], which is characteristic of an anisotropic behaviour [9].

The temperature variation of the strongest magnetic line is illustrated in Fig. 4. The ordering temperature is $T_N = 12(1)$ K and agrees well with reference [2].

DISCUSSION

$HoCo_2Si_2$ is a collinear antiferromagnet with $T_N = 12(1)$ K. The magnetic lattice is primitive P_I similar to the isomorphic $ErCo_2Si_2$ [5]. This means that the $\frac{111}{222}$ translation has become for the magnetic cell an anti-translation. The refinement of the 4.2 K magnetic data on the basis of a collinear model resulted in a magnetic moment direction along the c-axis. In this case the symmetry of the four fold axis does not get reduced (like in the case of $ErCo_2Si_2$). The magnetic space group is tetragonal: $I_P4/mm'm'$ or P_I4/mnc (Sh^{410}_{128}). The ordered Ho^{3+} moment is close to saturation value. The agreement between the observed and calculated data at 4.2 K was very good for this model. In addition the experimental magnetic form factor is very close to the theoretical curve [8]. From the refined parameters of Table 1 it is worth to be noted that the change of the $\Delta a/a_{293K}(\Delta a = a_{293K} - a_{4.2K})$ is larger by a factor 4 than for the c-axis. The silicon z parameter has also increased at 4.2 K.

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