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## A high-resolution neutron study of $\text{Y}_2\text{Fe}_{15}\text{Cr}_2$ at 77 K including magnetic properties

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**Abstract.** The crystallographic and magnetic structures of  $\text{Y}_2\text{Fe}_{15}\text{Cr}_2$  at 77 K have been refined by Rietveld analysis of the high-resolution neutron powder diffraction data. The analysis indicates that  $\text{Y}_2\text{Fe}_{15}\text{Cr}_2$  has  $\text{Th}_2\text{Ni}_{17}$ -type structure ( $P6_3/mmc$ ). The Cr atoms occupy 12j, 6g and 4f sites with occupancies 0.12, 0.10 and 0.50 respectively, but Cr atoms are absent at 12k sites. The magnetic moments of all of the magnetic atoms lie in the plane perpendicular to the sixfold axes and exhibit planar magnetic anisotropy. The relations between the interesting abnormal magnetic properties and the structure are discussed.

### 1. Introduction

In recent years, various magnetic materials based on  $\text{R}_2\text{Fe}_{17}$  have been extensively investigated in order to improve the magnetic properties. Two drawbacks restrict their application as permanent magnets: none of them exhibits an easy  $c$ -axis magnetocrystalline anisotropy at room temperature and the magnetic ordering temperature  $T_c$  of the compounds is relatively low. Therefore, many efforts have been made with the aim of solving such problems by either substituting other elements for iron in the  $\text{R}_2\text{Fe}_{17}$  structure or introducing interstitial atoms into the materials. It was found that the substitutions of the non-magnetic elements Al and Ga for Fe will increase the Curie temperature and change the easy-plane anisotropy to easy-axis anisotropy [1–5]. This paper reports the refined magnetic structure of  $\text{Y}_2\text{Fe}_{15}\text{Cr}_2$  at 77 K obtained using the high-resolution powder diffraction pattern. The refined structure shows that the Cr atoms occupy preferentially 12j, 6g and 4f sites with occupancies of 0.12, 0.10 and 0.50 respectively, and the magnetic moments of all of the magnetic atoms of the compound lie in the plane perpendicular to the sixfold axis and exhibit a ferromagnetic arrangement. The magnetic measurements indicate that the substitutions of Cr atoms lead to a slow decrease of the volume of the unit cell and an increase of the magnetic ordering temperature  $T_c$  with increasing Cr content  $x$  in the  $\text{Y}_2\text{Fe}_{17-x}\text{Cr}_x$  compounds. The magnetic ordering temperature  $T_c$  reaches a maximum (415 K) at approximately  $x = 1.0$ .

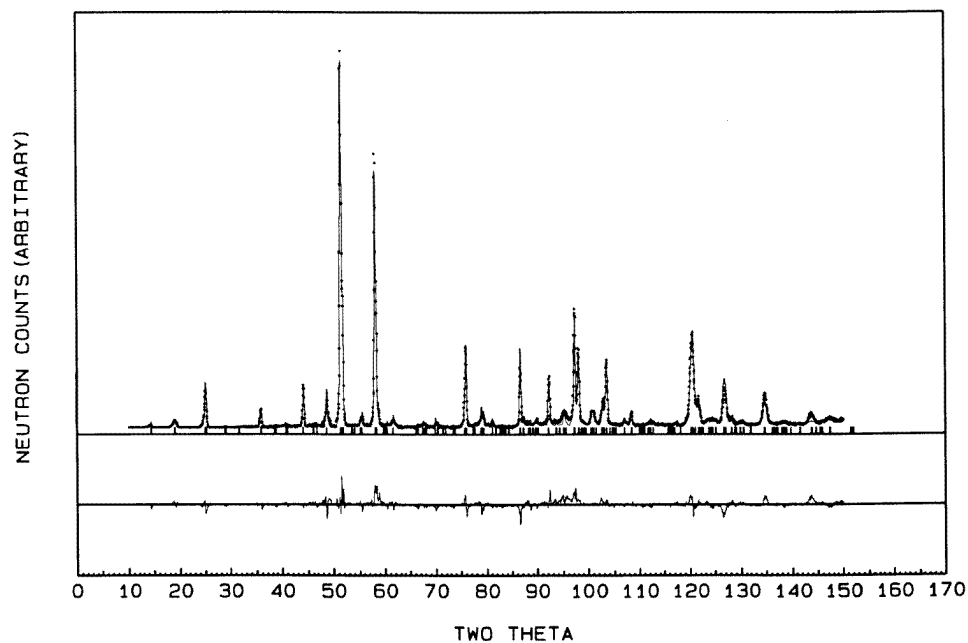
### 2. Experiments and refinements

The samples  $\text{Y}_2\text{Fe}_{15}\text{Cr}_2$  were prepared by arc melting high-purity Y (99.9% purity), Fe (99.95% purity) and Cr (99.9% purity) in an argon arc furnace and were annealed in a

**Table 1.** The magnetic ordering temperature  $T_c$ , saturation magnetization  $M_s$ , and unit-cell volume  $V$  as functions of the Cr content in  $Y_2Fe_{17-x}Cr_x$  compounds.

$x$	$T_c$ (K)	$M_s$ ( $\mu_B \text{ mol}^{-1}$ )	$V$ ( $\text{\AA}^3$ )
0	319	33.3	515.97
1	415	28.2	515.59
2	395	24.0	514.53
3	360	19.4	512.59
4	330	16.1	511.89

steel tube under an argon atmosphere at 1050 °C for 24 h. The ingots were then ground to yield powder samples. The samples were examined by x-ray diffraction. The results show that the samples have  $Th_2Ni_{17}$ -type structures (space group,  $P6_3/mmc$ ). The magnetic ordering temperature  $T_c$  was measured using the vibrating-sample magnetometer (VSM), the saturation magnetization  $M_s$  was measured using an extracting-sample magnetometer at 1.5 K under a field of 60 kOe, and the crystallographic unit-cell volume  $V$  was calculated from the x-ray pattern. The magnetic ordering temperatures  $T_c$ , the saturation magnetizations  $M_s$ , and the unit-cell volumes  $V$  of the  $Y_2Fe_{17-x}Cr_x$  compounds are listed in table 1.



**Figure 1.** The high-resolution powder diffraction pattern for  $Y_2Fe_{15}Cr_2$  at 77 K. The observed and calculated profiles are given by the dotted and solid curves respectively, and the calculated positions are indicated at the bottom. The differences between the observed and calculated data are also given.

Powder neutron diffraction was performed at 77 K by using a high-resolution powder diffractometer with a multi-detector system installed at Neutron Guide No 2 (NGT-2), at the Material Science Research Centre, attached to the Multi-Purpose Research Reactor, GA

Siwabessy (RSG-GAS), Serpong, Indonesia. The incident-neutron wavelength was 1.8215 Å monochromatized by the Ge(331) single crystal. The total (3200 points) data were collected by step scanning at 0.05° intervals over the angular range 2.5–162.5° with 32 detectors. The diffraction pattern is shown in figure 1. The collected data were analysed via the Rietveld structure refinement program RIETAN [6]. The parameters of the crystallographic structure of  $Th_2Ni_{17}$ -type rare-earth-iron compounds [7] were used to start the refinement. It was assumed that Fe and Cr atoms occupy simultaneously 6g, 12j, 12k, and 4f sites with the linear constraint condition: the sum of the occupancies of Fe and Cr atoms at each of the four sites equals 1.0. The possibilities of alignment of magnetic moments of Fe atoms either parallel or perpendicular to the sixfold axis were checked extensively in subsequent refinements.

Since the Cr atoms and Fe atoms occupy the same sites at random, their individual magnetic moments cannot be determined, so average moments for atoms in each of the 12j, 6g and 4f sites have been refined.

**Table 2.** Crystallographic and magnetic parameters of  $Y_2Fe_{15}Cr_2$  (space group  $P6_3/mmc$ ) at 77 K.  $a = 8.4124(8)$  Å;  $c = 8.3485(9)$  Å.

Atom	Occupancy	$x$	$y$	$z$	$B$ (Å <sup>2</sup> )	$M$ ( $\mu_B$ )
Y(2b)	1.00	0	0	0.25	0.87(9)	
Y(2d)	1.00	1/3	2/3	0.75	0.61(9)	
Fe(12k)	1.00	0.1648(2)	0.3296(3)	0.9894(5)	0.54(8)	2.1(2)
Fe(12j)	0.88(2)	0.3299(5)	−0.026(1)	0.25	0.97(3)	2.0(2)
Fe(6g)	0.90(2)	0.5	0	0	0.51(6)	2.0(2)
Fe(4f)	0.50(1)	1/3	2/3	0.1179(5)	1.1(1)	1.4(2)
Cr(12j)	0.12(2)	0.3299(5)	−0.026(1)	0.25	0.97(3)	2.0(2)
Cr(6g)	0.10(2)	0.5	0	0	0.51(6)	2.0(2)
Cr(4f)	0.50(3)	1/3	2/3	0.1179(5)	1.1(1)	1.4(2)

The refinements give a final  $R_{wp} = 12.5\%$ ; this is good for a high-resolution powder diffraction pattern with 3200 data points. The final refined crystallographic and magnetic parameters are listed in table 2. The magnetic moments of all of the magnetic atoms display ferromagnetic coupling and exhibit planar anisotropy. This is consistent with the x-ray diffraction results for magnetically aligned powders (the samples were ground to fine powders, mixed with epoxy resin and then oriented in an applied field of 10 kOe). The occupancies of Cr atoms on 12j, 6g and 4f sites agree with the Cr content in the compound.

### 3. Discussion

It is known that the volume of the unit cell expands and  $T_c$  increases simultaneously in  $R_2Fe_{17-x}T_x$  ( $T = Al$  and  $Ga$ ) compounds with increasing non-magnetic content  $x$  until  $x = 3.0$ , and then  $T_c$  decreases approximately linearly with increasing content  $x$ , continuously. In contrast, Yelon and co-workers [8] reported that the volume of the unit cell decreases and  $T_c$  increases simultaneously with increasing non-magnetic content  $x$  until  $x = 3.0$  in  $Nd_2Fe_{17-x}Si_x$  compounds and  $T_c$  decreases linearly with increasing  $x$ , continuously.

The results of magnetic measurements showed that the saturation magnetizations  $M_s$  of the compound show a linear dependence on Cr content  $x$ , because stronger magnetic Fe atoms were replaced by weaker magnetic Cr atoms. However, the relation between  $T_c$

and the Cr content  $x$  is of more interest: at first the Curie temperature  $T_c$  increases with increasing Cr content  $x$  until  $x = 1.0$ , and then  $T_c$  decreases approximately linearly with increasing Cr content  $x$ , continuously. There is a maximum of the Curie temperature at approximately  $x = 1.0$ . The refined structure of  $Y_2Fe_{15}Cr_2$  shows that the weaker magnetic atoms Cr occupy 12j, 6g and 4f sites with occupancies of 0.12, 0.10 and 0.50, respectively. It is known that there is an antiferromagnetic interaction between the Fe atoms at 4f sites, because the Fe–Fe bond length approaches 2.4 Å. The substitution of weaker magnetic atoms Cr for stronger magnetic atoms Fe on 4f sites may decrease the strength of the antiferromagnetic interactions at 4f sites and increase the total strength of the ferromagnetic interactions of the unit cell. The ferromagnetic exchange interactions directly affect the magnetic ordering temperature  $T_c$ ; therefore the substitution will increase the magnetic ordering temperature  $T_c$ . This may provide an explanation for the interesting relationship between  $T_c$  and the Cr content  $x$  in the  $Y_2Fe_{17-x}Cr_x$  compounds.

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### References

- [1] Hu Z, Yelon W B, Mishra S, Long G J, Pringle O A, Middleton D P and Buschow K H J 1994 *J. Appl. Phys.* **76** 443
- [2] Cheng Z H, Shen B G, Liang B, Zhang J X, Wang F W, Zhang S Y and Gong H Y 1995 *J. Phys.: Condens. Matter* **7** 4707
- [3] Hu B P and Coey J M D 1988 *J. Less-Common Met.* **142** 295
- [4] Gou C, Chen D F, Yan Q W, Zhang P L, Shen B G, and Cheng Z H 1995 *J. Phys.: Condens. Matter* **7** 837
- [5] Yelon W B, Xie H, Long G J, Pringle O A, Grandjean F and Buschow K H J 1993 *J. Appl. Phys.* **73** 6029
- [6] Izumi F 1985 *Kobutsugaku Zasshi* **17** 37
- [7] Buschow K H J 1977 *Rep. Prog. Phys.* **40** 1179
- [8] Long G J, Marasinghe G K, Mishra S, Pringle O A, Grandjean F, Buschow K H J, Middleton D P, Yelon W B, Pourarian F and Isnard O 1993 *Solid State Commun.* **88** 761