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$Ho_2Fe_{17-x}Al_xC(x=4$ and 7)

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Abstract. The crystallographic and magnetic structures of $Ho_2Fe_{17-x}Al_xC$ ($x = 4$ and 7) were investigated by powder neutron diffraction at room temperature. The results indicate that both compositions are isostructural with Th_2Zn_{17} (space group, $R\bar{3}m$). Aluminium substitutes for iron in three of the four Fe sites (18h, 18f and 6c in the hexagonal description of the rhombohedral cell) but not in 9d, and the fractional occupancies have been determined for both compositions. The carbon atoms occupy 9e sites. The saturation magnetization and Curie temperatures of samples with x in the range 0–7 are given; in the room-temperature magnetic structure of the phase with $x = 4$ the magnetic moments of all the atoms lie in the plane perpendicular to the $\bar{3}$ axis, with the Fe moments being ferrimagnetically coupled to those of Ho.

1. Introduction

In recent years, various magnetic materials based on R_2Fe_{17} (containing the interstitial atoms carbon, hydrogen and nitrogen) have been extensively investigated in order to improve magnetic properties [1–3]. Many studies have centred on either substituting other elements into the R_2Fe_{17} structure or preparing materials with additional atoms located interstitially. The substitution of other elements for Fe (e.g. Co, Al or Si) and the location of interstitial atoms (e.g. H, C or N) in R_2Fe_{17} will increase the Curie temperature [6, 9].

In order to understand the relation between the structure and magnetic properties, some studies of structure in $R_2Fe_{17-x}Al_xC$ have been made [1, 4–6, 8]. In this paper, the results of powder neutron diffraction measurements on $Ho_2Fe_{17-x}Al_xC$ ($x = 4$ and 7) are given, with the emphasis being placed on the site occupancies of the Al atoms. The saturation magnetization and Curie temperatures of samples with x in the range 0–7 are given and the room-temperature magnetic structure of the phase with $x = 4$ is described.

2. Experiment and refinement

The samples $Ho_2Fe_{17-x}Al_xC$ ($x = 4$ and 7) were prepared by arc melting high-purity Ho (99.9% purity), Fe–C alloy (99.9% purity) and Al (99.9% purity) in an argon arc furnace and were annealed in a steel tube under an argon atmosphere at 1150 °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 a Th_2Zn_{17}-type structure (space group, $R\bar{3}m$). The
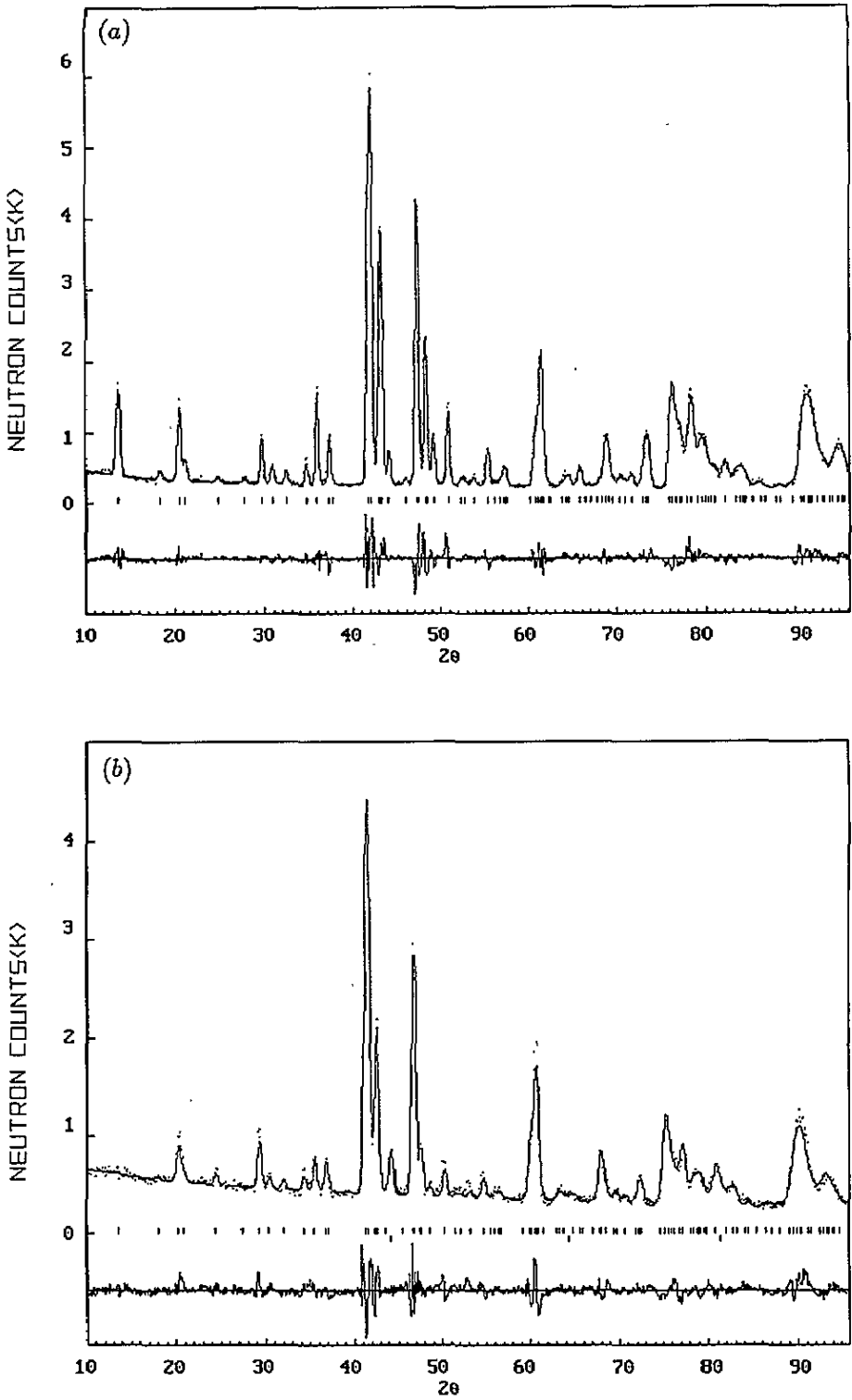
Figure 1. Final observed and calculated profiles: (a) Ho$_2$Fe$_{13}$Al$_4$C; (b) Ho$_2$Fe$_{10}$Al$_7$C.

magnetic measurements show that the sample with $x = 7$ exhibits paramagnetism at room temperature.

Powder neutron diffraction was performed on a triple-axis spectrometer at CIAE. The sample was contained in a vanadium can. The incident neutron wavelength was 1.541 Å from the (004) planes of a pyrolytic graphite monochromator. The analyser was pyrolytic graphite in the (002) setting. The collimation was 29′ in pile, 40′ monochromator–sample, 28′ sample–analyser and 40′ analyser–detector. The data were collected by step scanning at 0.1° intervals over the angular range 10–96°. The diffraction data were analysed by Izumi's [11] Rietveld structure refinement program RIETEN. The parameters of the crystallographic structure of Th$_2$Zn$_{17}$-type [10] rare-earth–iron compounds were used to start the refinement. It was assumed that the carbon atoms were on the 9e site [2, 3, 7], and the aluminium atoms and iron atoms occupy 18h, 18f, 9d and 6c sites simultaneously, according to chemical concentration and with the linear constraint condition; the sum of the occupancies of Fe and Al atoms on each of four sites equals 1. The magnetic moments of all magnetic atoms have a parallel arrangement and lie in a plane perpendicular to sixfold axes [10]. A small amount of α-iron was contained in the Ho$_2$Fe$_{10}$Al$_7$C sample; it was considered as the second phase in the refinement process.

The powder diffraction patterns are shown in figure 1. The crystallographic and magnetic parameters are listed in table 1. The magnetic moments of all iron atoms display ferromagnetic coupling, but the magnetic moments of Ho and Fe are antiferromagnetically oriented. The magnetic ordering temperature T_C of the compounds was measured with a vibrating-sample magnetometer; the Al concentration dependence of the Curie temperature is shown in figure 2. The magnetic ordering temperatures $T_C = 425$ and 260 K correspond to Al contents $x = 4$ and $x = 7$, respectively. The saturation magnetization (molecular) μ_S was measured using an extracting-sample magnetometer at 1.5 K, and μ_S versus Al content is shown in figure 3.
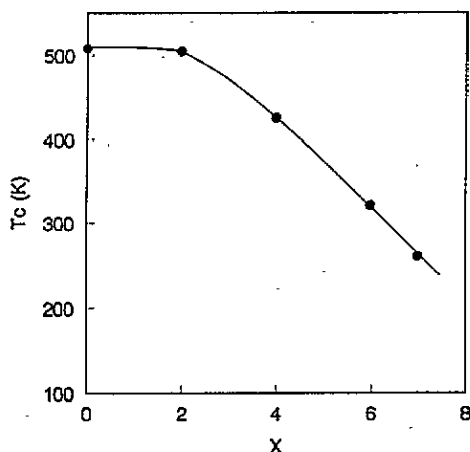

Figure 2. The dependence of the Curie temperature on the Al content x.
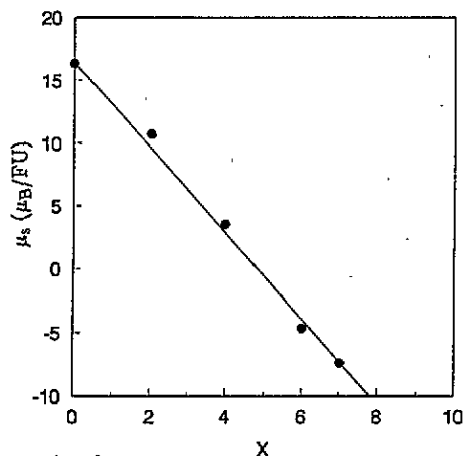

Figure 3. The saturation magnetization μ_S versus the Al content x at 1.5 K.

3. Discussion

The Rietveld structure analysis shows an obvious concentration dependence of the

Table 1. Crystallographic and magnetic parameters of $Ho_2Fe_{17-x}Al_xC$ ($x = 4$ and 7) (rhombohedral cell; space group; $R\bar{3}m$).

Atom	Wyckoff site	Occupancy factor	x	y	z	$M(\mu_B)$
		$x = 4$; $a = b = 8.648(1)$ Å; $c = 12.562(2)$ Å				
Ho	6c	1.0	0	0	0.341(2)	−3.63(45)
Fe	9d	1.0	0.5	0	0.5	−1.35(40)
Fe	18f	0.82(2)	0.286(1)	0	0	1.13(40)
Fe	18h	0.63(2)	0.503(1)	0.497(1)	0.154(1)	0.99(52)
Fe	6c	0.70(2)	0	0	0.096(2)	1.07(57)
Al	18f	0.18(2)	0.286(1)	0	0	
Al	18h	0.37(2)	0.503(1)	0.497(1)	0.154(1)	
Al	6c	0.30(2)	0	0	0.096(2)	
C	9e	0.33(3)	0.5	0	0	
		$x = 7$; $a = b = 8.745(2)$ Å; $c = 12.750(3)$ Å				
Ho	6c	1.0	0	0	0.347(3)	0
Fe	9d	1.0	0.5	0	0.5	0
Fe	18f	0.42(8)	0.289(2)	0	0	0
Fe	18h	0.69(9)	0.502(1)	0.498(1)	0.157(2)	0
Fe	6c	0.11(7)	0	0	0.100(4)	0
Al	18f	0.58(8)	0.289(2)	0	0	
Al	18h	0.31(9)	0.502(1)	0.498(1)	0.157(2)	
Al	6c	0.89(7)	0	0	0.100(4)	
C	9e	0.33(3)	0.5	0	0	

aluminium fractional occupancy on each of the four crystallographic sites (18h, 18f, 9d and 6c) in $Ho_2Fe_{17-x}Al_xC$ ($x = 4$ and 7). For $x = 4$, the aluminium atoms prefer the 18h site but, for $x = 7$, the aluminium atom population increased to 0.89 on the 6c site, and the occupancy of the 18f site is larger than that of 18h site. The 9d site excludes aluminium at two concentrations. All carbon atoms occupy the 9e site in the two samples. The lattice constants increase with increasing Al concentration, because the ion diameter of Al is larger than that of Fe. Similar results were obtained previously for the series $R_2Fe_{17-x}Al_x$ (R=Nd, Ho or Y) [1–4].

Figures 2 and 3 demonstrated that the magnetic ordering temperature T_C and the saturation magnetization μ_S decreased monotically when the Al content increases. However, for the saturation magnetization the decrease is linear with Al content, because magnetic Fe atoms were replaced by non-magnetic Al atoms and the magnetic moment of the Fe atoms stays approximately the same for the three sites (18h, 18f and 6c).

Acknowledgments

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