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Letter

The crystal structure and magnetic properties of the $GdCr_xAl_{12-x}$ ($x = 3.5$ and 4.0) intermetallics

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Abstract

The crystal structure of the $GdCr_xAl_{12-x}$ (with $x = 3.5$ and 4.0) intermetallic compound was determined by X-ray powder diffraction using the Rietveld method. The investigated compound crystallizes with $ThMn_{12}$ structure type (space group *I*4/*mmm*, Pearson symbol *tI*26). Magnetic measurements carried out for the title compound point to the antiferromagnetic–paramagnetic transition observed at $T_N = 6.50$ and 6.75 K for compositions with $x = 3.5$ and 4, respectively.

Keywords: Intermetallics; Crystal structure; X-ray diffraction; Magnetic properties

1. Introduction

Among the R–Cr–Al (R = Sc, Y and rare earths) ternary systems the isothermal sections were investigated in the partial or whole concentration region with R = Sc, Y, La, Ce, Gd, Dy, Yb [1–7]. Additionally, other alloys of these systems were investigated for the existence of the isostructural ternary compounds, which belong to the $CeCr_2Al_{20}$, $Ho_6Mo_4Al_{43}$ and $CeMn_4Al_8$ structure types [8–10]. Magnetic properties of some selected intermetallics of these systems were also studied [11,12].

In this paper, we report the results of crystal structure investigations of the $GdCr_xAl_{12-x}$ (with $x = 3.5$ and 4.0) intermetallic compound using the Rietveld method together with the results of magnetic measurements.

2. Experimental details

Samples were prepared by arc-melting of initial components under high purity argon on a water-cooled copper hearth. Starting materials were used in the form of pieces of high purity metals (>99.9 wt.%). The samples were remelted three times for a better homogeneity. Ingots were wrapped with tantalum foil and afterwards sealed in evacuated quartz tubes and annealed at 500 °C for 3 months. After heat treatment, the samples were quenched by submerging the silica tubes in cold water.

The crystal structures of ternary compounds were studied by means of X-ray powder diffraction (Siemens D500 diffractometer, Cu Kα-radiation, scanning parameters: 2θ region 10–145°, step scan 0.05°, counting time per step 10 s). All the crystal structure calculations were performed by means of the Rietveld method using the FullProf programme [13].

The magnetic susceptibility and magnetization of polycrystalline samples were determined by means of SQUID (Quantum Design) magnetometer, a Cahn RG automatic electro-balance and/or ac/dc magnetic measurements with Lake Shore 7225 apparatus in the temperature range from 2 to 300 K.

3. Results and discussion

The structure of the $GdCr_xAl_{12-x}$ (for $x = 3.5$ and 4.0) intermetallic compound annealed at 500 °C was refined from X-ray powder diffraction data using the Rietveld method. Pseudo-Voigt profile shape function was used. The background was refined with a polynomial function. The title ternary intermetallic compound crystallizes in tetragonal space group *I*4/*mmm* (Pearson symbol *tI*26), with $ThMn_{12}$ structure type (or $CeMn_4Al_8$ type with $x = 4.0$) [14]. The results of the crystal structure determination for the $GdCr_xAl_{12-x}$ with $x = 3.5$ and $x = 4.0$ are summarized in Table 1. Results of the Rietveld profile refinement of the $GdCr_4Al_8$ X-ray diffraction data are presented in Fig. 1. Projections of the $GdCr_xAl_{12-x}$ structure on the *xy* plane and coordination polyhedra for the atoms are given in Fig. 2. Interatomic distances and coordination numbers for atoms in the $GdCr_xAl_{12-x}$ are presented in Table 2. These dis-

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Table 1
Results of the crystal structure determination of the $GdCr_xAl_{12-x}$ ($x = 4.0$–3.5) compound

$GdCr_xAl_{12-x}$	$x = 3.5$	$x = 4.0$
Lattice parameters		
a (Å)	8.9900 (6)	8.9683(7)
c (Å)	5.1229 (4)	5.1252(5)
V (Å^3)	414.04 (5)	412.23(6)
Reliability factors		
R_B (%)	8.77	8.45
R_p (%)	3.31	3.39
Atom parameters		
	Gd in 2(a) 0 0 0	Gd in 2(a) 0 0 0
B_{iso} (Å^2)	0.68(10)	0.85(8)
	0.87(3)Cr + 0.13(3)Al in 8(f) 1/4 1/4 1/4	Cr in 8(f) 1/4 1/4 1/4
B_{iso} (Å^2)	0.67(13)	1.05(10)
	Al1 in 8(i) x 0 0	Al1 in 8(i) x 0 0
	$x = 0.3530(8)$	$x = 0.3537(8)$
B_{iso} (Å^2)	0.89(18)	0.46(18)
	Al2 in 8(j) x 1/2 0	Al2 in 8(j) x 1/2 0
	$x = 0.2791(8)$	$x = 0.2795(9)$
B_{iso} (Å^2)	0.64(18)	0.95(20)

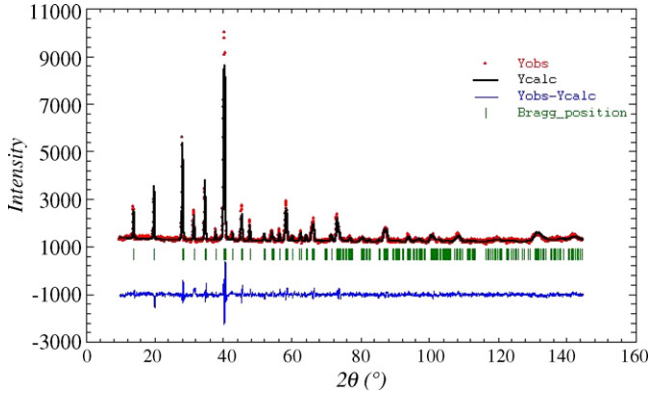

Fig. 1. Rietveld profile refinement of X-ray diffraction data for the $GdCr_4Al_8$.

Table 2
Interatomic distances (δ^*) and coordination numbers (CN) for atoms in the $GdCr_xAl_{12-x}$ intermetallics

Atoms	δ (Å)	CN	Atoms	δ (Å)	CN
$GdCr_xAl_{12-x}$ ($x = 3.5$)			$GdCr_xAl_{12-x}$ ($x = 4.0$)		
Gd		20	Gd		20
−4Al1	3.174		−4Al1	3.172	
−8Al2	3.241		−8Al2	3.237	
−8M	3.427		−8Cr	3.420	
M		12	Cr		12
−2Cr	2.561		−2Cr	2.563	
−4Al2	2.600		−4Al2	2.596	
−4Al1	2.748		−4Al1	2.745	
−2Gd	3.427		−2Gd	3.420	
Al1		14	Al1		14
−Al1	2.642		−Al1	2.624	
−4M	2.748		−4Cr	2.745	
−2Al2	2.824		−2Al2	2.827	
−2Al2	2.836		−2Al2	2.829	
−4Al1	3.170		−4Al1	3.164	
−Gd	3.174		−Gd	3.172	
Al2		12	Al2		12
−4M	2.600		−4Cr	2.596	
−2Al2	2.808		−2Al2	2.796	
−2Al1	2.824		−2Al1	2.827	
−2Al1	2.836		−2Al1	2.829	
−2Gd	3.241		−2Gd	3.237	

* Standard deviations ≤ 0.001 Å. M = 0.87(3)Cr + 0.13(3)Al.

tances are close to the sum of the atomic radii of the respective atoms.

SQUID magnetic measurements indicate that the $GdCr_xAl_{12-x}$ with $x = 3.5$ orders antiferromagnetically at Néel temperature $T_N = 6.50(5)$ K, presenting modified Curie–Weiss behaviour above T_N (Fig. 3a) in the form $\chi_\sigma = \chi_0 + C/(T - \Theta_p)$, where χ_0 is a temperature independent factor, C the Curie constant and Θ_p is the paramagnetic Curie temperature. The negative paramagnetic $\Theta_p = -5.9$ K Curie temperatures obtained for this composition of $GdCr_xAl_{12-x}$ compound points to a dominant antiferromagnetic exchange interaction among gadolinium magnetic moments. The effective magnetic moment

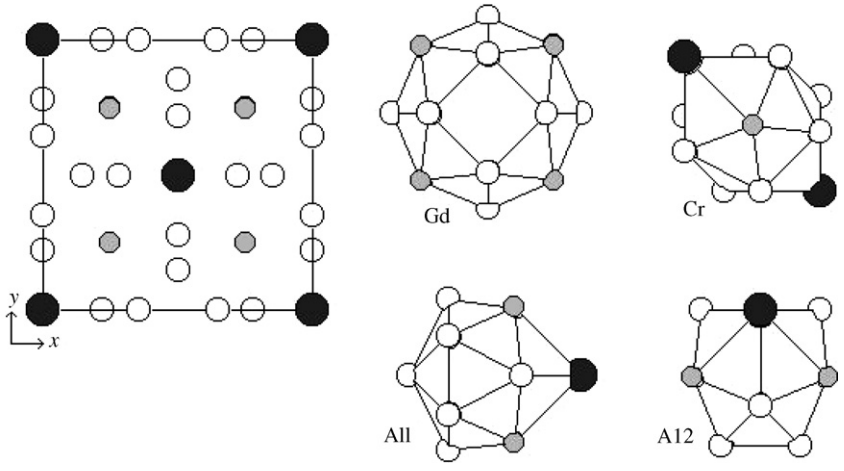

Fig. 2. Projections of the $GdCr_4Al_8$ structure on the xy plane and coordination polyhedra of the atoms. Black circles indicate Gd atoms, grey filled circles are Cr atoms, and Al atoms are marked by white circles.