Rietveld refinement of the crystal structures of hexagonal $Y_6Cr_{4+x}Al_{43-x}$ ($x=2.57$) and tetragonal $YCr_{4-x}Al_{8+x}$ ($x=1.22$)

R. Černý[a) and K. Yvon
Laboratoire de Cristallographie, Université de Genève, 24, quai Ernest-Ansermet, CH-1211 Geneva 4, Switzerland

T. I. Yanson, M. B. Manyako, and O. I. Bodak
Department of Inorganic Chemistry, L'viv University, 6, Lomonosova street, 290005 L'viv 5, Ukraine

$Y_6Cr_{4+x}Al_{43-x}$ ($x=2.57$); space group $P6_3/mcm$, $a=10.8601(1)$ Å, $c=17.6783(3)$ Å, $V=1805.7(1)$ Å^3, $Z=2$; isostructural to $Yb_6Cr_{4+x}Al_{43-x}$ ($x=1.76$) with two aluminium sites partially occupied by chromium (44% and 27% Cr). $YCr_{4-x}Al_{8+x}$ ($x=1.22$); space group $I4/mmm$, $a=9.0299(2)$ Å, $c=5.1208(2)$ Å, $V=417.55(3)$ Å^3, $Z=2$, disordered variant of $CeMn_4Al_8$ with one chromium site ($8f$) partially occupied by aluminium (33% Al); X-ray powder diffraction data were collected on a well-crystallized multiphase sample containing 43 wt. % of $Y_6Cr_{4+x}Al_{43-x}$, 27 wt. % of $Y_2Cr_{8-x}Al_{16+x}$, 16 wt. % of Al, 13 wt. % of YAl_3, and traces of Y_2O_3. Structure refinement converged at $R_{wp}=2.0\%$ and $R_B=3.5, 3.6\%$ resp. for a total of 78 parameters and 1190 reflections.

Key words: powder diffraction, Rietveld refinement, intermetallic phase

I. INTRODUCTION

An aluminium-rich ternary rare-earth (R) transition metal (T) phase of hexagonal symmetry and approximate composition $RTAl_8$ is known to occur in the systems $R=$ Y, Dy, Sm, Tb and $T=$ V, Cr (Zarechnyuk *et al.*, 1971; Rykhal' *et al.*, 1979; Zarechnyuk *et al.*, 1988). Its composition and structure was recently determined from single-crystal data on the representative in the Yb–Cr–Al system (Yanson *et al.*, 1994). The compound was described by the formula $Yb_6Cr_{4+x}Al_{43-x}$ ($x=1.76$) and found to contain an aluminium site which was partially occupied by chromium.

In this paper, we report on the structure refinement of another representative in the Y–Cr–Al system. As single crystals of sufficient quality were not available, the analysis was performed on a powder sample. The sample investigated was not single phase but contained significant amounts of other aluminides such as ternary YCr_4Al_8. The latter compound was previously studied by Zarechnyuk (1966) and described with the tetragonal $CeMn_4Al_8$ structure type, an ordered derivative structure of $ThMn_{12}$. In the present study the structure of YCr_4Al_8 was reinvestigated.

II. EXPERIMENTAL

A sample of nominal composition $YCrAl_7$ was prepared from the elements (Y: 99.9%, Cr: 99.99%, Al: 99.99% purity) by arc melting under argon atmosphere. The weight loss was less than 0.4%. No single crystals of satisfactory quality were found in the alloy. A powder sample was prepared by crushing the ingot, grinding in an agate mortar and sieving through a 50-μm (300-mesh) sieve. The powder was front-loaded in the sample holder ($20\times15\times0.5$ mm) of a Philips PW1820 powder diffractometer with Bragg–Brentano geometry (Ni-filtered CuK_α radiation; 35 kV, 40 mA). Diffraction

data were collected at room temperature in the 2θ range 7°–140° with a 2θ step width of 0.025° and a step time of 10 s (fixed divergency, scatter slits of 1°, receiving slit of 0.2 mm). Neither smoothing nor α_2 stripping was done. The background was approximated by a polynomial function and refined during Rietveld refinement. The zero point of the diffractometer was determined by an external Si standard (part of the Philips PW1769/00 alignement set, $a=5.4308$ Å).

III. STRUCTURE REFINEMENT

The sample contained five phases, hexagonal $Y_6Cr_{4+x}Al_{43-x}$ (space group $P6_3/mcm$), tetragonal YCr_4Al_8 ($I4/mmm$), rhombohedral YAl_3 ($R\bar{3}/m$), cubic Al
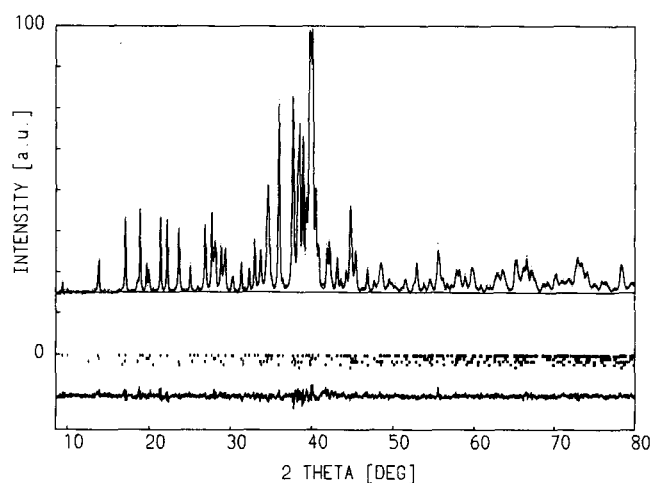

Figure 1. Observed (points), calculated (line) and difference (bottom of the figure) patterns of the Rietveld refinement. Only a part of pattern from $2\theta=8.60°$ to $2\theta=80°$ is shown. The refined background and line markers of the positions of Bragg peaks for all phases (from top down: $Y_6Cr_{4+x}Al_{43-x}$ ($x=2.57$), $YCr_{4-x}Al_{8+x}$ ($x=1.22$), YAl_3, Y_2O_3, and Al) are also given.

0885-7156/95/10(2)/86/5/$6.00

Phase	Weight fraction (%)
$Y_6Cr_{4+x}Al_{43-x}$	43(1)
$YCr_{4-x}Al_{8+x}$	27(1)
YAl_3	13(2)
Y_2O_3	1(0.2)
Al	16(1)

($Fm3m$), and traces of cubic Y_2O_3 ($Ia3$). For $Y_6Cr_{4+x}Al_{43-x}$ the reported parameters of $Yb_6Cr_{4+x}Al_{43-x}$ ($x=1.76$) were taken as a starting model for the structure refinement. For the other phases the refinement models were taken from a recent compilation of structure data (Villars and Calvert, 1991). The Rietveld code used was DBWS-9006PC (Wiles and Young, 1981). The atomic scattering factors and correction terms for anomalous dispersion were those included in the program. No correction for absorption was made.

During refinement it was found that some metal sites of the ternary compounds had mixed occupancies. In $Y_6Cr_{4+x}Al_{43-x}$ two aluminium sites were partially occupied by chromium. One, Al(6) (i.e., the same as that in the Yb compound), had an Al/Cr ratio of $\approx 1/1$ and the other, Al(7) (not partially occupied by Cr in the Yb compound), an Al/Cr ratio of $\approx 3/1$, corresponding to the refined composition $Y_6Cr_{4+x}Al_{43-x}$ ($x=2.57$). In YCr_4Al_8 the Cr site $8(f)$ is partially occupied by Al with an Al/Cr ratio of $\approx 1/2$, corresponding to the $YCr_{4-x}Al_{8+x}$ ($x=1.22$). The other two chromium sites $8(i)$ and $8(j)$ showed no evidence for mixed occupancy.

All phases showed weak preferred orientation with $(00.l)$ for $Y_6Cr_{4+x}Al_{43-x}$ and YAl_3, $(h00)$ for $Y_2Cr_{8-x}Al_{16+x}$ and (hhh) for Al and Y_2O_3 (planes parallel to

TABLE II. X-ray powder diffraction data for $Y_6Cr_{4+x}Al_{43-x}$ ($x=2.57$).

$h\,k\,l$	$2\theta_{obs}$ $CuK\alpha_1$ [deg]	d_{obs} [Å]	I_{obs}	I_{calc}
0 1 0	9.40	9.400	2	3
0 0 2	10.00	8.839	1	1
0 1 2	13.74	6.441	5	8
1 1 0	16.31	5.430	1	1
1 1 1	17.07	5.191	21	24
0 2 0	18.86	4.702	34	37
1 1 2	19.17	4.627	1	1
0 0 4	20.08	4.419	2	3
0 2 2	21.39	4.151	30	34
0 1 4 }	22.21	4.000	31	32
1 1 3 }				1
1 2 0	25.03	3.555	11	13
1 2 1	25.54	3.485	1	1
1 1 4	25.97	3.427	2	2
1 2 2	27.01	3.298	1	1
0 2 4	27.68	3.220	34	38
0 3 0	28.45	3.135	1	1
1 2 3	29.32	3.044	16	17
1 1 5 }	30.18	2.959	5	3
0 3 2 }				2
0 0 6	30.31	2.946	5	5
0 1 6	31.80	2.811	1	1
1 2 4	32.29	2.770	11	12
2 2 0	32.96	2.715	26	28
2 2 1	33.36	2.683	1	1
1 3 0	34.35	2.608	7	9
2 2 2 }	34.57	2.592	15	7
1 1 6 }				9
1 3 1	34.74	2.580	27	30
0 3 4	35.06	2.557	1	1
1 2 5 }	35.83	2.504	12	7
1 3 2 }				6
0 2 6	35.94	2.497	90	100
2 2 3	36.41	2.466	4	4
1 3 3	37.68	2.385	68	75
0 4 0	38.25	2.351	39	44
2 2 4	38.90	2.313	77	86
1 1 7	39.31	2.290	40	44
0 4 2 }	39.67	2.270	100	40
1 2 6 }				75
1 3 4	40.11	2.246	72	80
0 0 8	40.80	2.210	21	22
2 3 0	41.83	2.158	24	30
2 2 5 }	41.94	2.152	2	1
0 1 8 }				1
0 3 6	42.05	2.147	1	2
2 3 1	42.16	2.142	26	30
1 3 5 }	43.09	2.098	20	11
2 3 2 }				13
0 4 4	43.56	2.076	5	7
1 2 7	43.94	2.059	1	1
1 4 0	44.09	2.052	1	1
1 1 8	44.22	2.047	11	12
1 4 1	44.40	2.039	1	1
2 3 3	44.69	2.026	15	16
0 2 8 }	45.38	1.997	4	1
1 4 2 }				1
2 2 6 }				1
1 3 6 }				1
2 3 4 }	46.83	1.938	14	8
1 4 3 }				9
0 5 0	48.35	1.881	4	4
1 2 8	48.47	1.877	6	6
1 4 4	48.89	1.861	1	1
2 2 7 }	49.26	1.848	2	1
1 1 9 }				1
2 3 5 }	49.53	1.839	7	1
0 5 2 }				2
0 4 6 }				4
1 3 7	50.24	1.814	3	4
3 3 0	50.37	1.810	1	1
0 3 8	50.49	1.806	1	1
3 3 1	50.66	1.801	1	1
2 4 0 }	51.44	1.775	6	1
1 4 5 }				5
3 3 2 }				1
2 4 1 }	51.65	1.768	2	1
0 0 10 }				1

TABLE III. X-ray powder diffraction data for $YCr_{4-x}Al_{8+x}$ ($x=1.22$).

$h\ k\ l$	$2\theta_{obs}$ CuKα_1 [deg]	d_{obs} [Å]	I_{obs}	I_{calc}
1 1 0	13.86	6.385	17	19
0 2 0	19.65	4.515	17	17
0 1 1	19.92	4.454	13	13
2 2 0	27.92	3.192	21	22
1 2 1	28.12	3.171	33	33
1 3 0	31.30	2.855	23	21
0 3 1	34.54	2.595	53	50
0 0 2	35.02	2.560	4	4
1 1 2	37.83	2.376	2	2
0 4 0	39.90	2.257	100	100
2 3 1	40.04	2.250	84	85
0 2 2	40.47	2.227	80	78
3 3 0	42.44	2.128	8	10
2 4 0	44.85	2.019	20	20
1 4 1	44.98	2.014	1	1
2 2 2	45.37	1.997	33	34
1 3 2	47.67	1.906	10	9
1 5 0	51.57	1.771	5	4

the surface of the specimen). The following texture correction was applied (Čapková and Valvoda, 1974):

$$P_{hkl}(\alpha)=A\ \exp(-G\ \sin^2\ \alpha), \quad (1)$$

where α is the angle between the plane (hkl) and the preferrentialy oriented plane, and G is the refined parameter. The normalisation constant A was calculated from

$$1/4\pi\int_{4\pi}P_{hkl}\ d\Omega=1, \quad (2)$$

where Ω means an element of the solid angle. Because normalised texture correction conserves scattering matter/intensity (Hill, 1991), it was possible to estimate the weight fractions W_j of individual phases in the sample from the refined scale factors by

$$W_j=(SZMV)_j\bigg/\sum_j(SZMV)_j, \quad (3)$$

where $(SZMV)_j$ is a product of scale factor S, number of formula units per cell Z, mass per formula unit M and cell volume V of phase j. Results are given in Table I.

In the final stages of refinement, the following 78 parameters were allowed to vary: 21 atomic coordinates; 10 isotropic displacement parameters; 3 site occupation factors; 8 cell parameters; 1 sample displacement; 1 sample transparency parameter; 5 scale factors; 10 halfwidth; 3 asymmetry; 5 profile shape parameters; 5 texture parameters, and 6 background coefficients. The pseudo-Voigt profile function with Rietveld asymmetry parameter were used for all phases. The mixing parameter of the pseudo-Voigt function refined to values between 0.7 and 1.09 for the individual phases. The angular dependence of the peak full-width at half-maximum was described by the usual quadratic form. Refinement was based on the full pattern between 8.60 to 140° 2θ consisting of 650 and 138 reflections of the main phases $Y_6Cr_{4+x}Al_{43-x}$ and $YCr_{4-x}Al_{8+x}$, respectively, and 402 reflections for the minority phases. It converged at the following profile agreement factors: $R_{wp}=2.01\%$, $S=1.35$. The parameter of the weighted Durbin–Watson statistics ($d=1.19$) suggests positive serial correlations between adjacent residuals in the pattern ($Q=1.33$, see Hill and Flack, 1987). The Bragg agreement factors for the various phases are: $R_B=3.51\%$ ($Y_6Cr_{4+x}Al_{43-x}$), 3.61% ($YCr_{4-x}Al_{8+x}$), 1.45% (Al), 2.25% (YAl_3), and 5.24% (Y_2O_3).

The observed, calculated and difference patterns are represented in Figure 1. Powder diffraction data up to $2\theta=52°$ for $Y_6Cr_{4+x}Al_{43-x}$ and $YCr_{4-x}Al_{8+x}$ are given in the Tables II and III, respectively. Final atomic parameters for $Y_6Cr_{4+x}Al_{43-x}$ and $YCr_{4-x}Al_{8+x}$ are given in the Tables IV and V, respectively, and a comparison of selected interatomic distances of $Y_6Cr_{4+x}Al_{43-x}$ and $Yb_6Cr_{4+x}Al_{43-x}$ in Table VI.

IV. DISCUSSION

The structure of $Y_6Cr_{4+x}Al_{43-x}$ ($x=2.57$) can be seen as being formed from tenfold polyhedra around Cr(1) which are linked parallel to the hexagonal plane *via* common Al(7) atoms to groups of three (Figure 2). These units are linked perpendicular to the hexagonal plane *via* Cr(2) icosahedra to

TABLE IV. Atomic positional, displacement, and population parameters for $Y_6Cr_{4+x}Al_{43-x}$ ($x=2.57$).

Site	x	y	z	B_{iso} (Å^2)	Occup.
Y 12(k)	0.4663(2)	0	0.0961(1)	0.59(5)	
Cr(1) 6(g)	0.2596(5)	0	1/4	0.44(8)	
Cr(2) 2(b)	0	0	0	B_{iso}(Cr(1))[a]	
Al(1) 24(l)	0.2342(4)	0.3932(5)	0.1649(2)	0.60(7)	
Al(2) 12(k)	0.1562(5)	0	0.1178(4)	B_{iso}(Al(1))[a]	
Al(3) 12(k)	0.2613(7)	0	0.5291(4)	B_{iso}(Al(1))[a]	
Al(4) 12(j)	0.1522(7)	0.5480(8)	1/4	B_{iso}(Al(1))[a]	
Al(5) 12(i)	0.2501(8)	$2x$	0	B_{iso}(Al(1))[a]	
Al(6)[b] 8(h)	1/3	2/3	0.1333(3)	0.95(16)	Al:0.56(2) Cr:0.44(2)
Al(7)[b] 6(g)	0.8538(8)	0	1/4	B_{iso}(Al(6))[a]	Al:0.73(1) Cr:0.27(1)

[a] Constrained value.
[b] Mixed site, constrained to a total occupancy=1.
Space group $P6_3/mcm$ (No. 193), $a=10.8601(1)$ Å, $c=17.6783(3)$ Å, $V=1805.7(1)$ Å^3, $Z=2$.
$R_{wp}=2.01\%$, $S=1.35$, $R_B=3.51\%$ for 650 reflections.

TABLE V. Atomic positional, displacement and population parameters for $YCr_{4-x}Al_{8+x}$ ($x = 1.22$).

Site		x	y	z	B_{iso} (Å²)	Occup.
Y	2(a)	0	0	0	0.7(1)	
Cr[a]	8(f)	1/4	1/4	1/4	0.8(1)	Cr:0.67(1)
						Al:0.33(1)
Al(1)	8(i)	0.3402(6)	0	0	0.8(1)	
Al(2)	8(j)	0.2788(5)	1/2	0	B_{iso} (Al(1))[b]	

[a]Mixed site, constrained to a total occupancy = 1.
[b]Constrained value.

Space group $I4/mmm$ (No. 139), $a = 9.0299(2)$ Å, $c = 5.1208(2)$ Å, $V = 417.55(3)$ Å³, $Z = 1$.
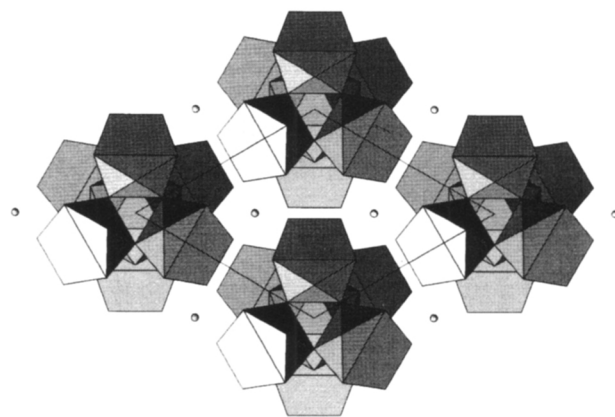$R_{wp} = 2.01\%$, $S = 1.35$, $R_B = 3.61\%$ for 138 reflections.

Figure 2. View of the $Y_6Cr_{4+x}Al_{43-x}$ ($x = 2.57$) structure in the [001] direction. Only Cr(1) polyhedra, Cr(2) icosahedra (positioned on the plane $z = 0$) and mixed occupied site Al(6) (circles) are drawn. Other atoms are omitted for clarity. The Cr(1) polyhedra are linked *via* common mixed occupied site Al(7).

columns along [001] at $x = 0$, $y = 0$. Adjacent columns are connected *via* mixed site Al(6) and Y atoms (not shown in Figure 2). The structures of $Y_6Cr_{4+x}Al_{43-x}$ ($x = 2.57$) and $Yb_6Cr_{4+x}Al_{43-x}$ ($x = 1.76$) differ mainly with respect to their cell dimensions and aluminium sites having mixed Al/Cr occupancy. (The estimated standard deviations of unit cell parameters are based only on the mathematics of Rietveld refinement. However, the unit cell parameter of Al impurity, $a = 4.0493(1)$ Å, corresponds very well to the literature data (Villars and Calvert, 1991). While the Yb compound has the smaller cell volume [$a = 10.867(1)$ Å,

$c = 17.554(2)$ Å, $V = 1795.3(3)$ Å³] and shows only one aluminium site with mixed occupancy [Al(6)], the Y compound has a larger cell volume [$a = 10.8601(1)$ Å, $c = 17.6783(3)$ Å, $V = 1805.7(1)$ Å³] and shows two aluminium sites with mixed occupancy, one [Al(6)] having about the same Cr/Al ratio of $\approx 1/1$ as the Yb compound, and another [Al(7)] having a Cr/Al ratio of $\approx 1/3$. The interatomic distances are consistent with these observations. All coordination polyhedra in the Y compound are bigger than those in the Yb compound, except for those of the mixed Al(7) site and the Cr(1) site which are smaller. In both compounds the separation between these sites is substantially smaller than the other Al–Cr distances in the structure. However, only in the Y compound is that separation, [Al(7) −Cr(1)] = 2.448 Å, consistent with possible Cr–Cr interactions.

The structure of $YCr_{4-x}Al_{8+x}$ ($x = 1.22$) has one chromium site, 8(f), which is partially occupied by aluminium (Figure 3), in contrast to the previous study (Zarechnyuk, 1966) in which that site was found to be fully occupied by Cr. One of the few other examples showing a preferential substitution on that site by a nontransition element is $LuFe_{10}Si_2$ (Buschow, 1988; Gueramian et al., 1991). In most other ternary $ThMn_{12}$ type derivatives, the substitution of the transition element occurs on the transition metal sites 8(i) and 8(j) (see Villars and Calvert, 1991; Gueramian et al., 1991). A compound whose structure can be derived from the tetragonal $CeMn_4Al_8$ structure type is $CaCr_2Al_{10}$ (Cordier et al., 1984). Aluminium in its structure substitutes half of the manganese on the 8(f) site such that an ordered superstructure with space group $P4/nmm$ is formed. No evidence of such an ordering in the present compound was found.

In conclusion, the present Rietveld analysis confirms that useful structural information can be obtained by this method on powder samples containing more than two phases and in the presence of rather complex atom arrangements. Our sample contained five different phases and the refinement converged for 34 atomic parameters to pattern consistency factors of $R_{wp} = 2.01\%$, $S = 1.35$ and Bragg intensity con-
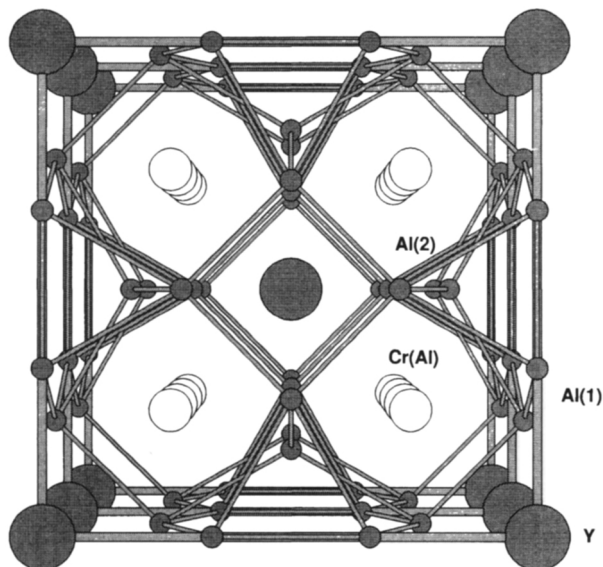
TABLE VI. Comparison of selected interatomic distances in $Y_6Cr_{4+x}Al_{43-x}$ ($x = 2.57$) and $Yb_6Cr_{4+x}Al_{43-x}$ ($x = 1.76$).

$Y_6Cr_{4+x}Al_{43-x}$ ($x = 2.57$) [powder, this work]			$Yb_6Cr_{4+x}Al_{43-x}$ ($x = 1.76$) [single crystal (Yanson et al., 1994)]		
Y			Yb		
	2Al(5)	3.066(7)		2Al(4)	3.044(6)
	2Al(1)	3.070(4)		2Al(5)	3.057(5)
	2Al(4)	3.075(8)		2Al(1)	3.062(4)
	Al(3)	3.139(6)		Al(3)	3.190(4)
	Al(3)	3.187(6)		2Al(6)	3.219(1)
	2Al(6)	3.225(2)		2Al(1)	3.232(8)
	2Al(1)	3.255(9)		Al(3)	3.270(4)
	2Al(5)	3.374(8)		2Al(5)	3.369(5)
	Al(2)	3.389(4)		Al(2)	3.389(4)
	Y	3.476(3)		Yb	3.444(1)
	Cr(1)	3.527(3)		Cr(1)	3.498(2)
Cr(1)			Cr(1)		
	2Al(7)	2.448(5)		2Al(7)	2.477(4)
	2Al(2)	2.593(7)		2Al(2)	2.638(5)
	4Al(1)	2.673(10)		4Al(1)	2.681(8)
	2Al(4)	2.714(9)		2Al(4)	2.681(6)
	2Y	3.527(3)		2Yb	3.498(2)
Cr(2)			Cr(2)		
	6Al(2)	2.686(6)		6Al(2)	2.635(6)
	6Al(3)	2.884(9)		6Al(3)	2.795(8)
Al(6)[a]			Al(6)[a]		
	3Al(1)	2.664(5)		3Al(1)	2.647(8)
	3Al(4)	2.693(10)		3Al(4)	2.732(12)
	3Al(5)	2.829(4)		3Al(5)	2.794(6)
	3Y	3.225(2)		3Yb	3.219(1)
Al(7)[a]			Al(7)		
	2Cr(1)	2.448(5)		2Cr(1)	2.477(4)
	2Al(7)	2.750(11)		4Al(1)	2.792(9)
	4Al(1)	2.794(8)		2Al(7)	2.827(9)
	4Al(2)	2.858(7)		4Al(2)	2.897(6)

[a]Also occupied by Cr.

Figure 3. View of the $YCr_{4-x}Al_{8+x}$ ($x = 1.22$) structure in the [001] direction.

Buschow, K. H. J. (**1988**). "Structure and properties of some novel ternary Fe-rich rare earth intermetallics," J. Appl. Phys. **63**, 3130–3135.

Čapková, P., and Valvoda, V. (**1974**). "Preferred orientation in powder samples of magnesium and magnesium-cadmium alloys," Czech. J. Phys. B **24**, 891–900.

Cordier, G., Czech, E., Ochmann, H., and Schäfer, H. (**1984**). "Neue übergangsmetallaluminide des Calciums," J. Less-Comm. Met. **99**, 173–185.

Gueramian, M., Yvon, K., and Hulliger, F. (**1991**). "Structure and magnetic properties of the $ThMn_{12}$-type compounds $RFe_{12-x}Re_x$ (R≡Ce-Nd, Sm, Gd-Tm, Lu, Y, Th, U)," J. Less-Comm. Met. **175**, 321–330.

Hill, R. J. (**1991**). "Expanded Use of the Rietveld Method in Studies of Phase Abundance in Multiphase Mixtures," Powder Diffr. **6**, 74–77.

Hill, R. J., and Flack, H. D. (**1987**). "The Use of the Durbin-Watson d Statistic in Rietveld Analysis," J. Appl. Cryst. **20**, 356–361.

Rykhal', R. M., Zarechnyuk, O. S., and Mats'kiv, O. P. (**1979**). "The isothermal section at 500 °C of the ternary systems Dy–V–Al and Dy–Cr–Al," Visn. L'viv Univ, Ser. Khim. **21**, 46–49.

Villars, P., and Calvert, L. D. (**1991**). *Pearson's Handbook of Crystallographic Data for Intermetallic Phases* (ASM International, Materials Park, OH 44073, USA).

Wiles, D. B., and Young, R. A. (**1981**). "A new computer program for Rietveld analysis of X-ray powder diffraction patterns," J. Appl. Cryst. **14**, 149; see also Sakthivel, A., and Young, R. A. (**1990**), *Program DBWS-9006* (School of Physics, Georgia Institute of Technology, Atlanta, GA 30332, USA).

Yanson, T. I., Manyako, M. B., Bodak, O. I., Zarechnyuk, O. S., Gladyshevskii, R. E., Černý, R., and Yvon, K. (**1994**). "Crystal structure of hexagonal $Yb_6Cr_{4+x}Al_{43-x}$ ($x = 1.76$)," Acta Cryst. C **50** (accepted).

Zarechnyuk, O. S. (**1966**). "The ternary compounds with superstructure from $ThMn_{12}$ type in the systems yttrium-transition metal–aluminium," Dopovidi Akad. Nauk Ukr. RSR **6**, 767–769.

Zarechnyuk, O. S., Rykhal, R. M., and German, N. V. (**1971**). "X-ray investigation of the alloys rich in aluminium in Y–V–Al and Y–Cr–Al systems," Visn. L'viv Univ., Ser. Khim. **12**, 10–12.

Zarechnyuk, O. S., Yanson, T. I., Ostrovskaya, O. I., and Shevchuk, L. P. (**1988**). "The isothermal section of the (Sm, Tb)-(V,Cr)-Al systems with the content of the Rare Earth Metals 0–0.33 at% at 770 K," Visn. L'viv Univ., Ser. Khim. **29**, 44–47.

sistency factors $R_B < 4\%$ for the two majority phases and $R_B < 6\%$ for the three minority phases. The error estimates of the atomic positions of one of the majority phases are only about three times higher compared to a single-crystal study on an isostructural compound. These results can be taken as further testimony for the potential of powder diffraction methods to investigate complex crystal structures and phase diagrams.