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The Crystal Structure of Orthorhombic $Gd_3Ni_5Al_{19}$, a New Representative of the Structure Series $R_{2+m}T_{4+m}Al_{15+4m}$

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The structure of $Gd_3Ni_5Al_{19}$ has been determined from single-crystal diffraction data [λ(Mo$K\alpha$) = 0.71073 Å, μ = 16.614 mm^{-1}, $F(000)$ = 2316, T = 293 K, wR = 0.023 for 997 contributing unique reflections]. This ternary aluminide crystallizes with a new, orthorhombic structure type, Pearson code $oS108$, (63) $Cmcm$, Wyckoff sequence $f^{12}c^3$, a = 4.0893(7), b = 15.993(2), c = 27.092(4) Å, V = 1771.8(5) Å^3, Z = 4, M_r = 1277.95, D_x = 4.790 mg mm^{-3}. The unit cell parameters of $GdNiAl_4$ with orthorhombic $YNiAl_4$ type, Pearson code $oS24$, (63) $Cmcm$, a = 4.0863(7), b = 15.520(4), c = 6.612(1) Å, were refined from single-crystal diffraction data [λ(Mo$K\alpha$) = 0.71073 Å, T = 293K]. The $Gd_3Ni_5Al_{19}$ structure can be considered as an intergrowth of two kinds of slab, one cut from the orthorhombic $YNiAl_4$ type and the second one corresponding to the translation unit of a hypothetical monoclinic $R_2T_4Al_{15}$ structure. The general formula of this inhomogeneous linear structure series can be expressed as $R_{2+m}T_{4+m}Al_{15+4m}$, where m is the number of consecutive intergrown $YNiAl_4$-type slabs. The $Gd_3Ni_5Al_{19}$ type is the simplest member of this structure series with m = 1. The following member with m = 2 is the monoclinic $Y_4Ni_6Al_{23}$ type.

Introduction

The structures of Al-rich compounds with rare-earth and transition metals are interesting since the majority of them are characterized by one short translation unit and particular coordination polyhedra: the rare-earth atoms center pentagonal (or hexagonal) prisms, the transition-metal atoms trigonal prisms, and the Al atoms distorted cubes (or pentagonal prisms).

In the Gd–Ni–Al system (0–40 at.% Gd) nine ternary phases have been observed at 1073 K by Rykhal', Zarechnyuk, and Marych (*1*), see also (*2*). Of the three compounds containing more than 50 at.% Al, the crystal structure was identified only for $GdNiAl_4$, which crystallizes in the orthorhombic $YNiAl_4$ type. An additional compound, $Gd_4Ni_6Al_{23}$ with monoclinic $Y_4Ni_6Al_{23}$ type, was recently found at lower temperature (773 K) by Gladyshevskii and Parthé (*3*). The structure determination of $Gd_3Ni_5Al_{19}$, a phase reported by Rykhal' *et al.* (*1*) as having nominal composition $GdNi_3Al_{16}$ and an orthorhombic cell, forms the subject of this paper.

Experimental

A sample of nominal composition $GdNi_3Al_{16}$ was prepared from Gd (99.9%), Ni

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(99.99%) and Al (99.99%) by arc-melting under argon atmosphere (weight loss 0.1%) and annealing at 1073 K for 2 weeks in a silica tube under an argon atmosphere (400 mm Hg). A single crystal [dimensions $\pm(100):0.064$ mm, $\pm(010):0.056$ mm, $\pm(001):0.024$ mm] was mounted on a Philips PW1100 automatic four-circle diffractometer (Mo$K\alpha$ radiation with graphite monochromator). The unit-cell parameters, refined from the 2θ values of 77 reflections (Mo$K\alpha$, $\lambda = 0.71073$ Å, $16° < 2\theta < 33°$), are in good agreement with those reported in (*1*, *2*). The 2534 reflections were collected out to $(\sin\theta/\lambda) = 0.702$ Å^{-1} ($0 \le h \le 5$, $0 \le k \le 16$, $0 \le l \le 38$ and the anti-reflections) in the ω-2θ scan mode, yielding 1218 unique reflections ($R_{int} = 0.041$). Maximum intensity variations of 1.2 and 1.0%, respectively, were observed for two standard reflections, 2 0 0 and $\bar{2}$ 0 0. Absorption correction was made using the program LSABS described in (*4*), max. and min. transmission factors were 0.6769 and 0.4203. The anomalous dispersion coefficients were taken from the "International Tables for X-ray Crystallography" (1974, Vol. IV). Systematic absences led to the following possible space groups: $Cmc2_1$, $C2cm$ (= $Ama2$), and $Cmcm$ ("International Tables for Crystallography," 1983, Vol. A). The structure was solved in space group $Cmcm$ by the MULTAN87 program (*5*) and confirmed by a structure refinement based on $|F|$ values. The 86 variables, including anisotropic atomic displacement parameters, were refined to $R = 0.032$ and $wR = 0.023$ [$w = 1/\sigma^2(|F_{rel}|)$, $S = 1.348$], considering 997 contributing unique reflections with $|F_{rel}| > 3\sigma(|F_{rel}|)$. Secondary extinction correction parameter (Gaussian distribution of mosaic spread) was refined to $G = 0.059(2)$. The max. shift/e.s.d. in the last cycle was 0.0005 and the final residual electron density $+3.3(-3.5)$eÅ^{-3}. The programs used to refine the structure are all from the XTAL3.0 system (*6*). The atomic positional parameters were standardized by using the STRUCTURE TIDY program (*7*). The atomic positional and displacement parameters are given in Table I[1] and the interatomic distances in Table II.

TABLE I

ATOMIC POSITIONAL AND DISPLACEMENT PARAMETERS FOR $Gd_3Ni_5Al_{19}$ WITH SPACE GROUP *Cmcm*

	Wyckoff position	x	y	z	U_{eq} (Å^2 × 100)
Al(1)	8(*f*)	0	0.0357(2)	0.6739(1)	1.1(1)
Ni(1)	8(*f*)	0	0.05368(9)	0.58406(5)	0.84(4)
Al(2)	8(*f*)	0	0.0676(2)	0.0309(1)	0.9(1)
Gd(1)	8(*f*)	0	0.16603(3)	0.13523(2)	0.68(2)
Al(3)	8(*f*)	0	0.2088(2)	0.5886(1)	0.9(1)
Al(4)	8(*f*)	0	0.2240(2)	0.6933(1)	1.0(1)
Al(5)	8(*f*)	0	0.2341(2)	0.0285(1)	0.9(1)
Ni(2)	8(*f*)	0	0.34076(8)	0.54208(5)	0.68(4)
Al(6)	8(*f*)	0	0.3700(2)	0.1349(1)	1.0(1)
Al(7)	8(*f*)	0	0.4055(2)	0.0374(1)	1.0(1)
Al(8)	8(*f*)	0	0.5366(2)	0.1008(1)	0.9(1)
Al(9)	8(*f*)	0	0.5786(2)	0.2017(1)	1.1(1)
Ni(3)	4(*c*)	0	0.0449(1)	¼	0.75(6)
Al(10)	4(*c*)	0	0.1926(3)	¼	1.1(2)
Gd(2)	4(*c*)	0	0.38709(5)	¼	0.67(2)

Note. The equivalent isotropic atomic displacement parameters are expressed as $U_{eq} = (\frac{1}{3})\Sigma_i\Sigma_j U_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j$. E.s.d.'s are given in parentheses.

Single crystals of $GdNiAl_4$ were found in a sample prepared in a similar way, but annealed at 773 K. The unit cell parameters were refined from the 2θ values of 20 reflections (Mo$K\alpha$, $\lambda = 0.71073$ Å, $19° < 2\theta < 34°$).

Discussion

The structure of $Gd_3Ni_5Al_{19}$ is shown in a projection along its short translation unit in the bottom row of Fig. 1. Two kinds of slab, parallel to the (0 0 1) plane, are emphasized on the drawing. The ~3.1-Å-thick slabs with polygons marked with dots have the composition $Gd_2Ni_2Al_8$. Stacking exclusively this

[1] Further details of the structure determination (e.g. structure factors) can be ordered from the Fachinformationszentrum Karlsruhe, D-7514 Eggenstein-Leopoldshafen (deposition N 370023).

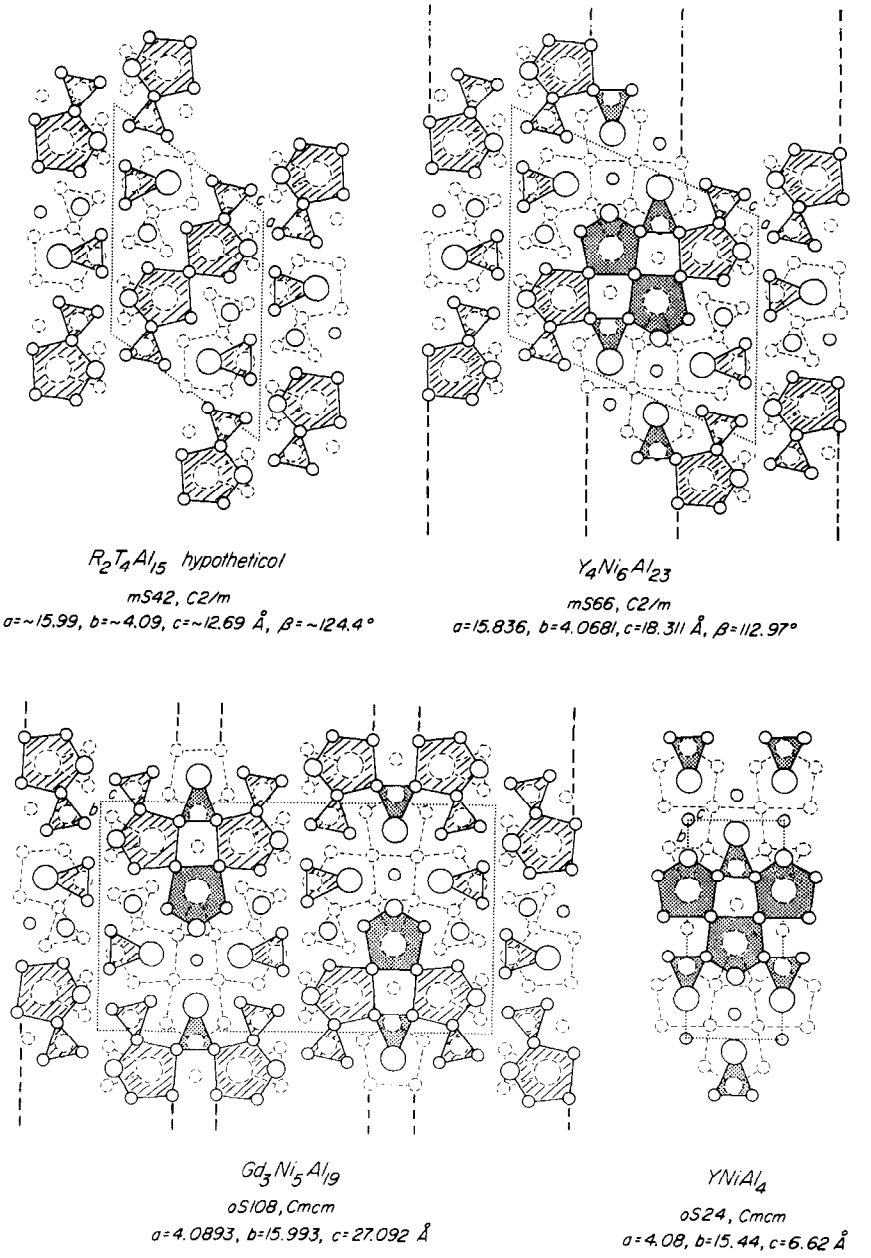

FIG. 1. Projections of $R_2T_4Al_{15}$ and $Y_4Ni_6Al_{23}$ along [0 1 0] and $Gd_3Ni_5Al_{19}$ and $YNiAl_4$ along [1 0 0]. Large circles, Y, Gd, or R; medium circles, Ni or T; and small circles, Al. The atoms drawn with full lines differ from those drawn with dashed lines by a shift of $\frac{1}{2}$ in height. The basal planes of the pentagonal and trigonal prisms at height $\frac{1}{2}$ in the $YNiAl_4$-type slabs are marked by dots, those in the $R_2T_4Al_{15}$-type slabs by stripes.

TABLE II

INTERATOMIC DISTANCES UP TO 4.0 Å IN $Gd_3Ni_5Al_{19}$

Gd(1)	2Al(8)	3.056(2)		2Al(8)	3.073(4)		2Al(3)	2.710(3)
	2Al(9)	3.063(3)		2Gd(2)	3.155(3)		2Ni(1)	2.751(2)
	Al(5)	3.091(3)		Gd(1)	3.393(3)		2Al(1)	2.751(3)
	2Al(4)	3.123(3)		Al(3)	3.606(5)		Al(8)	2.819(4)
	2Al(3)	3.129(3)	Al(2)	Ni(1)	2.416(4)		2Al(4)	2.992(4)
	Al(10)	3.138(1)		2Ni(2)	2.534(2)		Gd(2)	3.130(3)
	Al(2)	3.235(3)		Al(5)	2.664(5)		Gd(1)	3.262(3)
	2Ni(2)	3.250(1)		Al(2)	2.736(5)		Al(5)	3.611(5)
	Al(6)	3.262(3)		2Al(7)	2.791(3)		Al(9)	3.795(5)
	Al(1)	3.393(3)		2Al(8)	2.830(3)	Al(7)	Ni(2)	2.388(4)
	Ni(3)	3.663(1)		Ni(1)	3.123(4)		2Ni(1)	2.492(2)
	Ni(1)	3.777(2)		Gd(1)	3.235(3)		Al(6)	2.703(5)
Gd(2)	Al(10)	3.111(5)		2Al(7)	3.307(4)		Al(8)	2.711(5)
	4Al(4)	3.114(3)		Al(3)	3.947(5)		Al(5)	2.751(5)
	2Al(6)	3.130(3)	Al(3)	Ni(2)	2.459(4)		2Al(2)	2.791(3)
	4Al(1)	3.155(3)		Ni(1)	2.483(4)		2Al(3)	3.073(4)
	2Ni(3)	3.248(2)		2Al(6)	2.710(3)		2Al(2)	3.307(4)
	2Al(9)	3.330(3)		2Al(5)	2.769(3)		2Al(5)	3.514(4)
Ni(1)	Al(2)	2.416(4)		Al(4)	2.848(5)		Al(7)	3.638(5)
	Al(1)	2.452(4)		2Al(7)	3.073(4)		Al(8)	3.856(5)
	Al(3)	2.483(4)		2Gd(1)	3.129(3)	Al(8)	Ni(2)	2.525(3)
	2Al(7)	2.492(2)		Al(5)	3.197(5)		2Ni(1)	2.544(2)
	2Al(8)	2.544(2)		Al(1)	3.606(5)		Al(7)	2.711(5)
	2Al(6)	2.751(2)		Al(2)	3.947(5)		Al(9)	2.816(5)
	Al(2)	3.123(4)	Al(4)	Al(3)	2.848(5)		Al(6)	2.819(4)
	Gd(1)	3.777(2)		2Al(10)	2.884(3)		2Al(2)	2.830(3)
Ni(2)	Al(7)	2.388(4)		2Al(6)	2.992(4)		2Gd(1)	3.056(2)
	2Al(5)	2.398(2)		Al(1)	3.057(5)		2Al(1)	3.073(4)
	Al(3)	2.459(4)		Al(4)	3.070(5)		Al(7)	3.856(5)
	Al(8)	2.525(3)		2Gd(2)	3.114(3)	Al(9)	2Ni(3)	2.486(2)
	2Al(2)	2.534(2)		2Gd(1)	3.123(3)		Al(9)	2.615(5)
	Al(5)	2.562(4)		Al(9)	3.165(5)		Al(8)	2.816(5)
	2Gd(1)	3.250(1)	Al(5)	2Ni(2)	2.398(2)		2Al(1)	2.844(3)
Ni(3)	Al(10)	2.362(5)		Ni(2)	2.562(4)		2Al(10)	3.036(4)
	2Al(1)	2.431(3)		2Al(5)	2.611(3)		2Gd(1)	3.063(3)
	4Al(9)	2.486(2)		Al(2)	2.664(5)		Al(4)	3.165(5)
	2Gd(2)	3.248(2)		Al(7)	2.751(5)		Gd(2)	3.330(3)
	2Gd(1)	3.663(1)		2Al(3)	2.769(3)		Al(6)	3.795(5)
Al(1)	Ni(3)	2.431(3)		Gd(1)	3.091(3)	Al(10)	Ni(3)	2.362(5)
	Ni(1)	2.452(4)		Al(3)	3.197(5)		4Al(4)	2.884(3)
	2Al(6)	2.751(3)		2Al(7)	3.514(4)		4Al(9)	3.036(4)
	2Al(9)	2.844(3)		Al(6)	3.611(5)		Gd(2)	3.111(5)
	Al(4)	3.057(5)	Al(6)	Al(7)	2.703(5)		2Gd(1)	3.138(1)

Note. E.s.d.'s are given in parentheses.

kind of slab, one obtains the atom arrangement of the $GdNiAl_4$ structure, which crystallizes with the orthorhombic $YNiAl_4$ type (*8*), also shown in Fig. 1. The translation unit of $YNiAl_4$ contains two such slabs, rotated by 180° with respect to each other. The ~10.5-Å-thick slabs with polygons marked with stripes in the projection of $Gd_3Ni_5Al_{19}$

TABLE III

ATOMIC POSITIONAL PARAMETERS FOR $R_2T_4Al_{15}$: PEARSON CODE mS42, (12) $C2/m$, WYCKOFF SEQUENCE $i^{10}c$, $a \simeq 15.99$, $b \simeq 4.09$, $c \simeq 12.69$ Å, $\beta \simeq 124.4°$, $Z = 2$[a]

	Wyckoff position	x	y	z
$T(1)$	4(i)	0.044	0	0.218
Al(1)	4(i)	0.103	0	0.080
Al(2)	4(i)	0.106	0	0.771
Al(3)	4(i)	0.188	0	0.479
Al(4)	4(i)	0.267	0	0.074
R	4(i)	0.323	0	0.350
Al(5)	4(i)	0.449	0	0.097
Al(6)	4(i)	0.526	0	0.349
Al(7)	4(i)	0.654	0	0.261
$T(2)$	4(i)	0.708	0	0.109
Al(8)	2(c)	0	0	½

[a] For a definition of the Pearson code and the Wyckoff sequence, see (*12*) and (*7*), respectively.

have the composition $Gd_4Ni_8Al_{30}$. These slabs form a monoclinic $R_2T_4Al_{15}$ structure, shown in the top row of Fig. 1, when stacked by simple translation. Crystallographic data for this structure type, which has not yet been observed, are given in Table III. The numerical values have been calculated from those observed for $Gd_3Ni_5Al_{19}$.

The $Gd_3Ni_5Al_{19}$ type is the simplest member ($n = 1$, $m = 1$) of an inhomogeneous linear structure series of general formula $R_{2n+m}T_{4n+m}Al_{15n+4m}$, where n is the number of $R_2T_4Al_{15}$-type slabs intergrown with m $YNiAl_4$-type slabs. A member of this structure series with $n = 1$ and $m = 2$ was identified as monoclinic $Y_4Ni_6Al_{23}$ (*9*), which can be seen in a projection along [0 1 0] in Fig. 1. Since for both the $Gd_3Ni_5Al_{19}$ and $Y_4Ni_6Al_{23}$ types $n = 1$, the formula of the structure series can be simplified to $R_{2+m}T_{4+m}Al_{15+4m}$. Members with $m > 2$ are as yet unknown, however, it is possible to build structure models, considering a simple intergrowth of m consecutive $YNiAl_4$-type slabs with one $R_2T_4Al_{15}$-type slab. It appears that for m odd, the intergrowth structure will have orthorhombic symmetry (space group $Cmcm$), whereas for m even, the intergrowth structure will be monoclinic (space group $C2/m$). The cell parameters for any simple member with $n = 1$ of this structure series can be calculated from the cell parameters of the parent structures (a', b', c', β' refer to the $R_2T_4Al_{15}$ type and $a'' \simeq b'$, $b'' \simeq a'$, c'' to the $YNiAl_4$ type) by applying the following equations:

for m odd ($Cmcm$)

$$a \simeq b'$$
$$b \simeq a'$$
$$c \simeq 2c' \cdot \sin\beta' + m \cdot c'',$$

for m even ($C2/m$)

$$a \simeq a'$$
$$b \simeq b'$$
$$c \simeq \sqrt{(c')^2 + (m \cdot c''/2)^2 + m \cdot c' \cdot c'' \cdot \sin\beta'}$$
$$\beta \simeq \operatorname{arctg}\,[(2c' \cdot \sin\beta' + m \cdot c'')/(2c' \cdot \cos\beta')].$$

Cell parameters for $Gd_3Ni_5Al_{19}$, $Gd_4Ni_6Al_{23}$, and $GdNiAl_4$ are given in Table IV. Corresponding values for hypothetical structures with $m = 0$, $m = 3$, and $m = 4$, calculated from the values observed for the known members in the Gd–Ni–Al system, have been added. It is observed that the longest translation unit of the slabs (a for monoclinic and b for orthorhombic structures) decreases with increasing number of consecutive intergrown $YNiAl_4$-type slabs (from 16.0 to 15.5 Å).

A related intergrowth structure has been observed for $U_4Ni_5Al_{18}$ (*10*), where three $YNiAl_4$-type slabs of composition $U_2Ni_2Al_8$ are intergrown with ~4.7-Å-thick slabs of composition $U_2Ni_4Al_{12}$ (see drawing in (*9*)). The latter can be obtained by cutting slabs of the hypothetical $R_2T_4Al_{15}$ structure discussed above.

Both the $YNiAl_4$-type and the $R_2T_4Al_{15}$-

TABLE IV

CRYSTALLOGRAPHIC CHARACTERISTICS FOR SIMPLE MEMBERS AND PARENT STRUCTURES OF THE INHOMOGENEOUS SERIES $R_{2n+m}T_{4n+m}Al_{15n+4m}$ IN THE Gd–Ni–Al SYSTEM

Composition	n	m	Pearson code	Space group	Wyckoff sequence	a (Å)	b (Å)	c (Å)	β (°)
"$Gd_2Ni_4Al_{15}$"	1	0	$mS42$	$C2/m$	$i^{10}c$	15.99	4.09	12.69	124.4
$Gd_3Ni_5Al_{19}$	1	1	$oS108$	$Cmcm$	$f^{12}c^3$	4.0893	15.993	27.092	
$Gd_4Ni_6Al_{23}$	1	2	$mS66$	$C2/m$	$i^{16}c$	15.856	4.078	18.286	113.01
"$Gd_5Ni_7Al_{27}$"	1	3	$oS156$	$Cmcm$	$f^{18}c^3$	4.09	15.73	40.78	
"$Gd_6Ni_8Al_{31}$"	1	4	$mS90$	$C2/m$	$i^{22}c$	15.62	4.09	24.76	106.8
$GdNiAl_4$	0	1	$oS24$	$Cmcm$	fc^3a	4.0863	15.520	6.612	

Note. Compounds at compositions placed between quotation marks have not yet been observed.

type slabs can be considered as an arrangement of R-centered pentagonal prisms and T-centered trigonal prisms. The basal planes at height $\frac{1}{2}$ of these polyhedra are marked with dots or stripes, Fig. 1. It is possible to include information on the partial coordinations in the general crystal-chemical formula[2] for a ternary compound $R_xT_yM_z$. As an extension to the originally proposed use of the crystal-chemical formula, containing information about individual coordinations, we shall consider here average partial coordination numbers:

$$R_x^{[r_T,r_M;r_R]}T_y^{[t_R,t_M;t_T]}M_z^{[m_R,m_T;m_M]}.$$

Taking into account that

$$xr_T = yt_R, \quad xr_M = zm_R, \quad \text{and } yt_M = zm_T,$$

one can rewrite it in the following way:

$$R_x^{[r_T,r_M;r_R]}T_y^{[(x/y)r_T,t_M;t_T]}M_z^{[(x/z)r_M,(y/z)t_M;m_M]}.$$

Since the pentagonal prisms around the R atoms are formed by two T atoms and eight Al atoms and there are no T atoms at the vertices of the trigonal prisms, the crystal-chemical formula for the structure series discussed above becomes

$$R_x^{[(2,8)p;0]}T_y^{[(2x/y,6-2x/y)p;0]}M_z^{[8x/z,6y/z-2x/z;m_M]}. \tag{1}$$

It should be noted that atoms are not considered here, which are located in the same atom layer, perpendicular to the short translation axis, as the central atoms even if some of the interatomic distances are of the same magnitude. The average number of Al–Al contacts between the central Al atoms and the surrounding ones (m_M) will be derived from geometrical considerations. It can indeed be shown that for structures built up of two kinds of monoatomic layer where the atoms of one layer center all polygons of the other layer, the average number of coordinating atoms belonging to neighbouring layers, is equal to 8. The more general equation,

$$m_M = [8(x + y + z) - x(r_T + 2r_M + r_R) - y(t_R + 2t_M + t_T)]/z,$$

[2] Coordination symbols are added to the symbols of the chemical elements as trailing superscripts and placed between square brackets. Symbols before a semicolon refer to the heteronuclear coordination (r_T, r_M for R; t_R, t_M for T; m_R, m_T for M) and those after it to the homonuclear coordination (r_R, t_T and m_M). The shape of the coordination polyhedron can further be indicated by a small letter (p stands for prism and cb for a cube) where the number (or the sum of the numbers) before the letter indicates the number of vertices (*11*).

may, by inserting the values which are characteristic of the $R_{2+m}T_{4+m}Al_{15+4m}$ structure series, be simplified to

$$m_M = 4(2 - 2x/z - y/z). \qquad (2)$$

After calculating the average partial coordinations of the T and the Al atoms for each individual structure from Eqs. (1) and (2), the crystal-chemical formulas for the two known members and the parent structures can be expressed as

$$R_2^{[(2,8)p;0]}T_4^{[(1,5)p;0]}Al_{15}^{[16/15,4/3;88/15]}$$
$$Gd_3^{[(2,8)p;0]}Ni_5^{[(6/5,24/5)p;0]}Al_{19}^{[24/19,24/19;108/19]}$$
$$Y_4^{[(2,8)p;0]}Ni_6^{[(4/3,14/3)p;0]}Al_{23}^{[32/23,28/23;128/23]}$$
$$Y^{[(2,8)p;0]}Ni^{[(2,4)p;0]}Al_4^{[2,1;5]}.$$

It is now possible to find the polyhedra around the Al sites from the sum of the partial average coordination numbers for Al. Due to the presence of a mirror plane through the atom layers perpendicular to the short translation axis, only polyhedra with an even number of vertices need be considered. Furthermore, polyhedra with less than eight vertices are highly unlikely for Al atoms in rare earth–transition metal aluminides. In the case of $Gd_3Ni_5Al_{19}$ the average number of neighbours around the Al sites is (24 + 24 + 108)/19 = 156/19. It follows that of the 19 Al atoms in the formula unit, 17 center cubes and the remaining 2 center pentagonal prisms: 17 · 8 + 2 · 10 = 156. For $Y_4Ni_6Al_{23}$, with the average number of atoms surrounding the Al sites being equal to 188/23, 21 Al atoms center cubes and 2 Al atoms center pentagonal prisms: 21 · 8 + 2 · 10 = 188. The polyhedra obtained in this way are in good agreement with the observed ones:

$$R_2^{[(2,8)p;]}T_2^{[(2,4)p;]}T_2^{[,6p;]}Al_{13}^{[8cb]}Al_2^{[10p]}$$
$$Gd_3^{[(2,8)p;]}Ni_3^{[(2,4)p;]}Ni_2^{[,6p;]}Al_{17}^{[8cb]}Al_2^{[10p]}$$
$$Y_4^{[(2,8)p;]}Ni_4^{[(2,4)p;]}Ni_2^{[,6p;]}Al_{21}^{[8cb]}Al_2^{[10p]}$$
$$Y^{(2,8)p;]}Ni^{[(2.4)p;]}Al_4^{[8cb]}.$$

As already stated above, in order to get the actual coordinations, additional atoms should be taken into account. When these atoms are included the coordination numbers increase to 15, 9–10, and 12–14 for the rare-earth, transition-metal, and Al atoms, respectively.

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