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The first aluminide with $Ho_4Ni_{10}Ga_{21}$-type structure

Svitlana PUKAS[1]*, Pavlo DEMCHENKO[1], Roman GLADYSHEVSKII[1]

[1] *Department of Inorganic Chemistry, Ivan Franko National University of Lviv, Kyryla i Mefodiya St. 6, 79005 Lviv, Ukraine*
* *Corresponding author. Tel.: +380-32-2394506; e-mail: s_pukas@franko.lviv.ua*

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Tetralutetium decanickel henicosaaluminide, $Lu_4Ni_{10}Al_{21}$, was synthesized by arc melting and its crystal structure was studied by X-ray powder diffraction. It is isotypic to $Ho_4Ni_{10}Ga_{21}$: Pearson symbol *mS*70, space group *C*2/*m*, *a* = 20.7920(4), *b* = 4.0279(1), *c* = 15.4778(3) Å, *β* = 124.878(1)°. The structure of the $Lu_4Ni_{10}Al_{21}$ compound belongs to a family of two-layer structures, where the atoms of each layer are situated at the centers of straight prisms built of atoms of the neighboring layers. The Lu and Ni atoms center pentagonal and trigonal prisms, respectively, whereas the Al atoms center square and pentagonal prisms in the ratio 15:6 in this description.

Aluminum / Lutetium / Nickel / X-ray powder diffraction / Crystal structure / Crystal-chemical formulae

Introduction

15 representatives of the monoclinic structure type $Ho_4Ni_{10}Ga_{21}$ (Pearson symbol *mS*70, space group *C*2/*m* [1]) are known so far according to Pearson's Crystal Data [2]. They are rare-earth nickel gallides $R_4Ni_{10}Ga_{21}$ (*R* = Y, Tb, Dy, Ho, Er, Tm, Yb, and Lu [1]) and rare-earth or thorium palladium indides $R_4Pd_{10}In_{21}$ (*R* = La, Ce, Pr, Nd, Sm [3], Gd [4], and Th [5]). Complete rows of isotypic compounds with respect to the rare earths do not exist for any of the above mentioned groups: the heavy rare-earth elements form ternary compounds with nickel and gallium, whereas the light rare-earth elements form compounds with palladium and indium (Table 1). A substitution variant of the $Ho_4Ni_{10}Ga_{21}$ type is $U_4Ni_{11}Ga_{20}$ [6]. It has 7 representatives in the systems U–{Ni,Pd,Pt}–Ga [6] and {Y,Gd,Tb,Dy}–Ni–In [7,8]. The absence of compounds isotypic to $Ho_4Ni_{10}Ga_{21}$ or $U_4Ni_{11}Ga_{20}$ with aluminum, *e.g.* in *R*–Ni–Al systems, is unexpected.

In 1982, Rykhal' *et al.* [9] reported that the ternary systems *R*–Ni–Al (*R* = Y, Gd-Tm, and Lu) are characterized by the formation of a ternary compound of nominal composition ~$R_2Ni_3Al_7$ with unknown structure. Later the structure of the compound with Gd was solved from X-ray single-crystal diffraction data: own structure type $Gd_3Ni_7Al_{14}$, Pearson symbol *hP*72, space group *P*-62*m*, *a* = 17.966(5), *c* = 4.0448(6) Å [10]. Other compounds with the same stoichiometry (except *R* = Lu) appeared to be isotypic to $Gd_3Ni_7Al_{14}$ [11,12].

In this work we present the results of a structural investigation of a new ternary lutetium nickel aluminide, $Lu_4Ni_{10}Al_{21}$. In the Lu–Ni–Al system the existence of eight compounds has been reported [13] (Table 2). The structure of the equiatomic compound belongs to the hexagonal ZrNiAl-type structure, while its high-pressure modification belongs to the hexagonal $MgZn_2$-type structure. To our best knowledge, a structure determination of the compound with nominal composition ~$Lu_2Ni_3Al_7$ had not been carried out up to now.

Experimental

An alloy of nominal composition $Lu_{12.5}Ni_{29.2}Al_{58.3}$ ($Lu_3Ni_7Al_{14}$) of total mass 1 g was synthesized from high-purity metals (Lu ≥ 99.83 wt.%, Ni ≥ 99.99 wt.%, and Al ≥ 99.998 wt.%) by arc-melting in a water-cooled copper crucible under a purified argon atmosphere, using Ti as a getter and a tungsten electrode. To achieve high efficiency of the interaction between the components, the sample was melted twice. The ingot was annealed at 600°C under vacuum in a quartz ampoule for 1 month and subsequently quenched in cold water.

The phase and structural analyses were performed based on X-ray powder diffraction data collected on a diffractometer STOE STADI P (Cu $K\alpha_1$ radiation, wavelength λ = 1.5406 Å) in the angular range $4 \le 2\theta \le 110.545°$ with the step 0.015° and scan time 250 s.

Table 1 Ternary compounds with the $Ho_4Ni_{10}Ga_{21}$- or $U_4Ni_{11}Ga_{20}$-type structure.

Compound	Y	La	Ce	Pr	Nd	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu	Th	U
$R_4Ni_{10}Ga_{21}$	+								+	+	+	+	+	+	+		
$R_4Ni_{11}Ga_{20}$																	+
$R_4Pd_{11}Ga_{20}$																	+
$R_4Pt_{11}Ga_{20}$																	+
$R_4Ni_{11}In_{20}$	+							+	+	+							
$R_4Pd_{10}In_{21}$		+	+	+	+	+		+								+	

Table 2 Crystallographic parameters of compounds reported in the Lu–Ni–Al system.

Compound	Structure type	Pearson symbol	Space group	*a*, Å	*b*, Å	*c*, Å	Ref.
Lu_3Ni_8Al	Ce_3Co_8Si	*hP*24	$P6_3/mmc$	4.985	–	15.940	[9]
Lu_2Ni_2Al	W_2CoB_2	*oI*10	*Immm*	4.124	5.263	8.253	[9]
LuNiAl	ZrNiAl	*hP*9	*P*-62*m*	6.906	–	3.748	[9]
LuNiAl	$MgZn_2$	*hP*12	$P6_3/mmc$	5.280	–	8.491	[14]
$LuNiAl_2$	$MgCuAl_2$	*oS*16	*Cmcm*	4.038	9.875	6.900	[9]
$LuNi_2Al_3$	YNi_2Al_3	*hP*18	*P*6/*mmm*	9.000	–	4.032	[9]
$Lu_2Ni_3Al_7$	...	*hP*...	...	17.850	–	4.044	[9]
$LuNiAl_4$	$YNiAl_4$	*oS*24	*Cmcm*	4.023	14.970	6.630	[9]
$Lu_3Ni_5Al_{19}$	$Gd_3Ni_5Al_{19}$	*oS*108	*Cmcm*	3.924	15.400	26.540	[9]

The structure was refined by the Rietveld method, using the program DBWS-9807 [15]. The structure drawings were made with the program ATOMS [16].

Results and discussion

As can be seen from Table 3, where the results of the X-ray phase analysis are shown, the alloy used for the structural analysis, $Lu_{12.5}Ni_{29.2}Al_{58.3}$, was a two-phase sample and contained, in addition to the new phase $Lu_4Ni_{10}Al_{21}$ (86.9(4) wt.%), the phase $LuNiAl_2$ (13.1(8) wt.%), which was known before [9]. In the final cycle of the refinement, 58 parameters were allowed to vary: zero shift, scale factor for each phase, four and three cell parameters, respectively, for the two phases, five profile parameters (pseudo-Voigt function), 34 and four positional parameters for $Lu_4Ni_{10}Al_{21}$ and $LuNiAl_2$, respectively, three displacement parameters, and one texture parameter for each phase. The isotropic displacement parameters for the same chemical element were constrained to be equal for both compounds.

Experimental details and crystallographic data are presented in Table 3. Atomic coordinates and isotropic displacement parameters for $Lu_4Ni_{10}Al_{21}$ are given in Table 4, interatomic distances are listed in Table 5. A projection of the unit cell of the structure of the new compound along the crystallographic direction [010], and conventional coordination polyhedra, are presented in Fig. 1. Atomic coordinates for $LuNiAl_2$ are given in Table 6.

In the structure of $Lu_4Ni_{10}Al_{21}$ the Lu atoms occupy two Wyckoff positions, the Ni atoms five and the Al atoms eleven positions. The Lu atoms from both sites have similar environment: a pentagonal prism consisting of four Ni and six Al atoms. Five rectangular faces of these prisms are capped exclusively by Al atoms, whereas the bases of the prisms are capped by Lu atoms; three additional Ni atoms are situated above the lateral edges of the prisms. The Ni atoms center trigonal prisms consisting of six Al atoms (site Ni1), or two Lu and four Al atoms (sites Ni2, Ni3, Ni4, and Ni5), with additional atoms of different kinds. In the case of site Ni1, the coordination polyhedron includes six additional atoms: three Al atoms are situated above rectangular faces and one Ni and two Lu atoms above side edges of the trigonal prisms. In the case of sites Ni2, Ni3, and Ni4 there are five additional atoms: one Lu and four Al, two Lu and three Al, and one Lu, one Ni and three Al atoms, respectively. The smallest number of additional atoms is observed for the atoms from site Ni5: one Ni and three Al atoms. In all cases the rectangular faces of the trigonal prisms are capped exclusively by Al atoms, whereas Lu, Ni, and/or additional Al atoms are situated above the edges. Prisms are also observed as coordination polyhedra for the Al atoms, which center pentagonal (site Al3: composition Al_{10}), square (sites Al2 and Al11: Ni_4Al_4, sites Al4, Al5, Al6, Al7, Al9, and Al10: $Lu_2Ni_2Al_4$), as well as trigonal (sites Al1 and Al8: Ni_2Al_4) prisms. These prisms are capped by 4-5 additional atoms of different kinds.

The $Ho_4Ni_{10}Ga_{21}$-type structure belongs to a family of two-layer structures, which are characterized by at least one short cell parameter [17]. Table 7 lists 28 types that form in the systems *R*–*T*–Al, where *R* is

Table 3 Details of the structural refinement of $Lu_4Ni_{10}Al_{21}$ and $LuNiAl_2$.

Compound		$Lu_4Ni_{10}Al_{21}$	$LuNiAl_2$
Content, wt.%		86.9(4)	13.1(8)
Structure type		$Ho_4Ni_{10}Ga_{21}$	$MgCuAl_2$
Space group		*C*2/*m*	*Cmcm*
Cell parameters:	*a*, Å	20.7920(4)	4.0475(1)
	b, Å	4.0279(1)	9.8550(4)
	c, Å	15.4778(3)	6.8180(2)
	β, º	124.878(1)	
Cell volume *V*, Å^3		1063.40(4)	271.95(2)
Formula units per cell *Z*		2	4
Density D_X, g cm^{-3}		5.791	7.028
Scale factor		$0.126(1)\cdot 10^{-4}$	$0.238(2)\cdot 10^{-4}$
Texture parameter *G* [direction]		1.031(2) [100]	1.092(7) [010]
Number of reflections		842	118
Reliability factor R_B		0.0731	0.0644
FWHM parameters *U*, *V*, *W*		0.050(3), -0.013(2), 0.012(1)	
Mixing parameter η		0.655(8)	
Asymmetry parameter C_M		-0.073(6)	
Number of refined parameters		58	
Reliability factors R_p, R_{wp}		0.0647, 0.1010	
Goodness of fit *S*		1.00	

Table 4 Atom coordinates and isotropic displacement parameters for $Lu_4Ni_{10}Al_{21}$: structure type $Ho_4Ni_{10}Ga_{21}$, *mS*70, *C*2/*m*, *a* = 20.7920(4), *b* = 4.0279(1), *c* = 15.4778(3) Å, *β* = 124.878(1)º.

Site	Wyckoff position	*x*	*y*	*z*	B_{iso}, Å^2
Lu1	4*i*	0.1204(2)	0	0.3324(2)	0.41(2)
Lu2	4*i*	0.7695(2)	0	0.1741(2)	
Ni1	4*i*	0.0255(4)	0	0.6051(5)	
Ni2	4*i*	0.1346(5)	0	0.1021(6)	
Ni3	4*i*	0.2553(4)	0	0.6178(6)	0.66(6)
Ni4	4*i*	0.3444(4)	0	0.1112(5)	
Ni5	4*i*	0.5065(4)	0	0.1881(5)	
Al1	4*i*	0.0076(8)	0	0.0910(9)	
Al2	4*i*	0.0549(7)	0	0.7847(9)	
Al3	4*i*	0.1183(8)	0	0.5484(9)	
Al4	4*i*	0.2000(8)	0	-0.0073(9)	
Al5	4*i*	0.2517(8)	0	0.2975(9)	
Al6	4*i*	0.3025(9)	0	0.5008(9)	1.11(7)
Al7	4*i*	0.3885(8)	0	0.2987(9)	
Al8	4*i*	0.4027(8)	0	0.0051(9)	
Al9	4*i*	0.5358(8)	0	0.3675(9)	
Al10	4*i*	0.6278(8)	0	0.1921(9)	
Al11	2*d*	0	½	½	

a rare-earth element and *T* is a *d*-element of group VIII of the periodic system. In these structures the atoms of each layer are situated at the centers of straight prisms, which are built up of atoms of the neighboring layers. The axes of the prisms are parallel to the short translation period. In the $Ho_4Ni_{10}Ga_{21}$-type structure the layers (nets of triangles, squares and pentagons) are situated at $y = 0$ and $y = ½$ and, because of the *C*-translation, each atom site is alternatively centering and forming the prisms. It should be noted that this description increases the number of vertices of the polyhedra around sites Al1 (instead of a Ni_2Al_4 trigonal prism, we now consider a Ni_2Al_6 square prism including two additional Al atoms at 3.59 Å), Al2 (instead of a Ni_4Al_4 square prism, we now consider a Ni_4Al_6 pentagonal prism including two additional Al atoms at 3.48 Å), and Al8 (instead of a Ni_2Al_4 trigonal prism, we now consider a Ni_2Al_8 pentagonal prism including four additional Al atoms at 3.48 and 3.59 Å).

Table 5 Interatomic distances in $Lu_4Ni_{10}Al_{21}$.

Atoms		*δ*, Å
Lu1	-2 Al9	2.922(14)
	-2 Al6	2.925(8)
	-2 Ni5	2.933(4)
	-1 Al2	3.002(13)
	-2 Ni3	3.009(7)
	-2 Al10	3.029(13)
	-1 Al5	3.071(20)
	-1 Al1	3.072(11)
	-1 Al6	3.137(14)
	-1 Al3	3.368(17)
	-1 Ni3	3.635(8)
	-1 Ni1	3.674(11)
	-1 Ni2	3.741(12)
	-2 Lu1	4.0279(1)
Lu2	-2 Al7	2.905(9)
	-2 Al5	2.941(13)
	-1 Al4	2.990(19)
	-1 Al8	3.026(12)
	-2 Ni4	3.027(8)
	-2 Al4	3.064(9)
	-2 Ni2	3.097(8)
	-1 Al10	3.114(19)
	-1 Al2	3.328(16)
	-1 Al3	3.526(12)
	-1 Ni3	3.541(12)
	-1 Ni4	3.626(7)
	-1 Ni1	3.632(6)
	-2 Lu2	4.0279(1)
Ni1	-2 Al11	2.449(4)
	-1 Al2	2.482(17)
	-2 Al7	2.535(8)
	-1 Al3	2.536(22)
	-1 Al3	2.542(13)
	-2 Al9	2.545(13)
	-1 Ni1	2.786(11)
	-1 Lu2	3.632(6)
	-1 Lu1	3.674(11)
Ni2	-2 Al8	2.437(9)
	-2 Al10	2.498(12)
	-1 Al1	2.546(22)
	-1 Al5	2.579(12)
	-1 Al4	2.711(23)
	-1 Al1	2.751(12)
	-2 Lu2	3.097(8)
	-1 Lu1	3.741(12)
Ni3	-1 Al3	2.402(18)
	-2 Al5	2.452(12)
	-1 Al6	2.505(23)
	-2 Al6	2.519(8)
	-1 Al10	2.527(12)
	-2 Lu1	3.009(7)
	-1 Lu2	3.541(12)
	-1 Lu1	3.635(8)

Atoms		*δ*, Å
Ni4	-2 Al4	2.408(7)
	-1 Al4	2.466(15)
	-1 Al7	2.494(16)
	-1 Al8	2.538(22)
	-2 Al2	2.679(8)
	-1 Ni5	2.862(11)
	-2 Lu2	3.027(8)
	-1 Lu2	3.626(7)
Ni5	-1 Al8	2.385(12)
	-1 Al9	2.479(17)
	-1 Al10	2.487(21)
	-2 Al1	2.521(12)
	-2 Al2	2.545(12)
	-1 Ni4	2.862(11)
	-2 Lu1	2.933(4)
Al1	-2 Ni5	2.521(12)
	-1 Ni2	2.546(22)
	-1 Al1	2.649(23)
	-2 Al8	2.695(12)
	-1 Ni2	2.751(12)
	-1 Al2	2.872(26)
	-2 Al10	2.877(13)
	-1 Lu1	3.072(11)
Al2	-1 Ni1	2.482(17)
	-2 Ni5	2.545(12)
	-2 Ni4	2.679(8)
	-2 Al9	2.843(10)
	-1 Al1	2.872(26)
	-1 Al4	2.891(14)
	-2 Al7	2.974(19)
	-1 Lu1	3.002(13)
	-1 Lu2	3.328(16)
Al3	-1 Ni3	2.402(18)
	-1 Ni1	2.536(22)
	-1 Ni1	2.542(13)
	-2 Al11	2.926(12)
	-2 Al6	2.963(21)
	-2 Al9	3.057(12)
	-2 Al5	3.111(11)
	-2 Al7	3.172(19)
	-1 Lu1	3.368(17)
	-1 Lu2	3.526(12)
Al4	-2 Ni4	2.408(7)
	-1 Ni4	2.466(15)
	-1 Ni2	2.711(23)
	-2 Al4	2.809(18)
	-1 Al2	2.891(14)
	-2 Al8	2.950(19)
	-1 Lu2	2.990(19)
	-2 Lu2	3.064(9)

Atoms		*δ*, Å
Al5	-2 Ni3	2.452(12)
	-1 Ni2	2.579(12)
	-1 Al6	2.686(20)
	-1 Al7	2.834(26)
	-2 Al10	2.924(13)
	-2 Lu2	2.941(13)
	-1 Lu1	3.071(20)
	-2 Al3	3.111(11)
Al6	-1 Ni3	2.505(23)
	-2 Ni3	2.519(8)
	-1 Al5	2.686(20)
	-1 Al9	2.761(20)
	-2 Lu1	2.925(8)
	-2 Al6	2.960(21)
	-2 Al3	2.963(21)
	-1 Lu1	3.137(14)
Al7	-1 Ni4	2.494(16)
	-2 Ni1	2.535(8)
	-1 Al9	2.605(23)
	-1 Al11	2.612(10)
	-1 Al5	2.834(26)
	-2 Lu2	2.905(9)
	-2 Al2	2.974(19)
	-2 Al3	3.172(19)
Al8	-1 Ni5	2.385(12)
	-2 Ni2	2.437(9)
	-1 Ni4	2.538(22)
	-2 Al1	2.695(12)
	-1 Al10	2.739(22)
	-2 Al4	2.950(19)
	-1 Lu2	3.026(12)
Al9	-1 Ni5	2.479(17)
	-2 Ni1	2.545(13)
	-1 Al11	2.551(18)
	-1 Al7	2.605(23)
	-1 Al6	2.761(20)
	-2 Al2	2.843(10)
	-2 Lu1	2.922(14)
	-2 Al3	3.057(12)
Al10	-1 Ni5	2.487(21)
	-2 Ni2	2.498(12)
	-1 Ni3	2.527(12)
	-1 Al8	2.739(22)
	-2 Al1	2.877(13)
	-2 Al5	2.924(13)
	-2 Lu1	3.029(13)
	-1 Lu2	3.114(19)
Al11	-4 Ni1	2.449(4)
	-2 Al9	2.551(18)
	-2 Al7	2.612(10)
	-4 Al3	2.926(12)

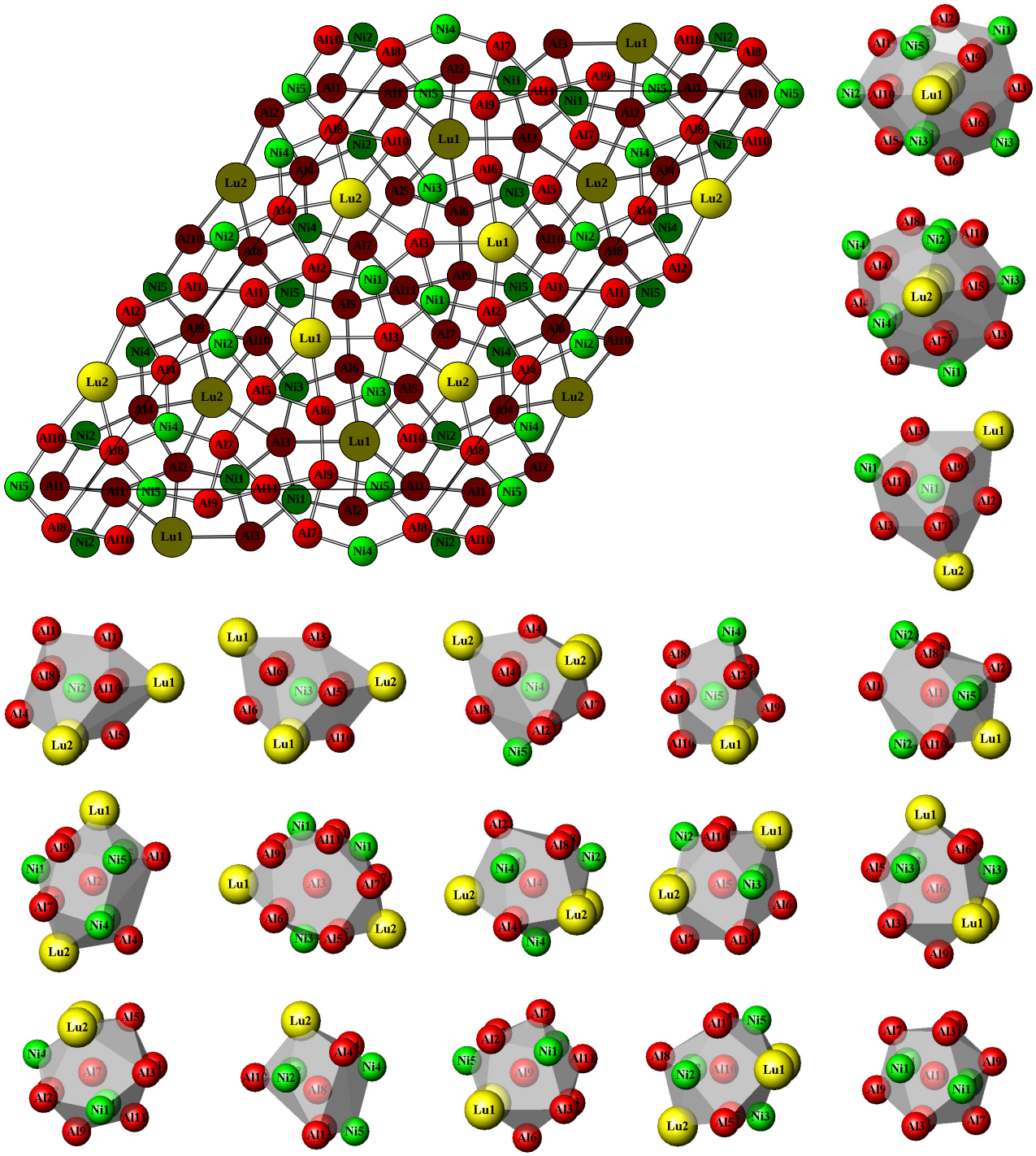

Fig. 1 Projection of the structure of $Lu_4Ni_{10}Al_{21}$ along [010] (nets of triangles, squares and pentagons at y = 0 and y = ½ are indicated) and conventional coordination polyhedra.

Table 6 Atom coordinates and isotropic displacement parameters for $LuNiAl_2$: structure type $MgCuAl_2$, *oS*16, *Cmcm*, a = 4.0475(1), b = 9.8550(4), c = 6.8180(2) Å.

Site	Wyckoff position	x	y	z	B_{iso}, Å^2
Lu	4*c*	0	0.4332(5)	¼	0.41(2)
Ni	4*c*	0	0.7072(11)	¼	0.66(6)
Al	8*f*	0	0.1481(13)	0.0440(15)	1.11(7)

Table 7 "Two-layer structure types" represented in the systems {Sc,Y,La,*Ln*,*Ac*}–{Fe,Co,Ni}–Al: Pearson symbol, space group and the types of straight prism (number of vertices in square brackets) centered by the rare-earth, transition metal and Al atoms, respectively. Crystallographic data can be found in [2].

Structure type	Pearson symbol	Space group	*R*	*T*	Al
$BaFe_2Al_9$	*hP*12	*P*6/*mmm*	$[12]_1$	$[6]_2$	$[8]_9$
$CeFe_2Al_8$	*oP*44	*Pbam*	$[10]_1$	$[6]_2$	$[8]_7[10]_1$
$Gd_3Ni_5Al_{19}$	*oS*108	*Cmcm*	$[10]_3$	$[6]_5$	$[8]_{17}[10]_2$
YNi_5Si_3	*oP*36	*Pnma*	$[12]_1$	$[6]_3$	$[8]_4[10]_1$
$Ho_4Ni_{10}Ga_{21}$	*mS*70	*C*2/*m*	$[10]_4$	$[6]_{10}$	$[8]_{15}[10]_6$
$Y_4Ni_6Al_{23}$	*mS*66	*C*2/*m*	$[10]_4$	$[6]_6$	$[8]_{21}[10]_2$
$PrNi_2Al_5$	*oI*16	*Immm*	$[12]_1$	$[6]_2$	$[8]_5$
$ZrNi_2Al_5$	*tI*16	*I*4/*mmm*	$[8]_1$	$[8]_2$	$[8]_5$
$Gd_3Ni_7Al_{14}$	*hP*72	*P*-62*m*	$[10]_1[12]_2$	$[6]_7$	$[8]_{12}[10]_2$
$U_4Ni_5Al_{18}$	*mS*54	*Cm*	$[10]_4$	$[6]_5$	$[8]_{17}[10]_1$
$LaCoAl_4$	*oP*12	*Pmma*	$[10]_1$	$[6]_1$	$[8]_4$
$YNiAl_4$	*oS*24	*Cmcm*	$[10]_1$	$[6]_1$	$[8]_4$
$UCoAl_4$	*hP*18	*P*-62*m*	$[10]_1$	$[6]_1$	$[8]_4$
$PrNi_2Al_3$	*hP*6	*P*6/*mmm*	$[12]_1$	$[6]_2$	$[8]_3$
YNi_2Al_3	*hP*18	*P*6/*mmm*	$[12]_1$	$[6]_2$	$[8]_3$
YCo_3Ga_2	*hP*18	*P*6/*mmm*	$[12]_1$	$[6]_2[8]_1$	$[8]_2$
$YNiAl_3$	*oP*20	*Pnma*	$[10]_1$	$[6]_1$	$[8]_3$
$Ce_3Pt_4Al_6$	*oP*52	*Pnma*	$[10]_1[12]_2$	$[6]_4$	$[6]_1[8]_5$
$MgCuAl_2$	*oS*16	*Cmcm*	$[10]_1$	$[6]_1$	$[8]_2$
$Ce_3Co_3Al_4$	*oP*40	*Pnma*	$[10]_3$	$[6]_3$	$[8]_4$
CePdAl	*oP*42	*Pmmn*	$[10]_1$	$[6]_1$	$[8]_1$
CeCoAl	*mS*12	*C*2/*m*	$[10]_1$	$[6]_1$	$[8]_1$
TiNiSi	*oP*12	*Pnma*	$[10]_1$	$[6]_1$	$[8]_1$
LaNiAl	*oP*24	*Pnma*	$[10]_1$	$[6]_1$	$[8]_1$
ZrNiAl	*hP*9	*P*-62*m*	$[10]_1$	$[6]_1$	$[8]_1$
$Pr_7Co_6Al_7$	*tP*40	*P*4/*mbm*	$[8]_1[10]_6$	$[6]_6$	$[8]_7$
W_2CoB_2	*oI*10	*Immm*	$[10]_2$	$[6]_2$	$[8]_1$
Mo_2FeB_2	*tP*10	*P*4/*mbm*	$[10]_2$	$[6]_2$	$[8]_1$

The crystal-chemical formulae [18] of ternary aluminides with the $Ho_4Ni_{10}Ga_{21}$-type structure can be written as follows, considering only the atoms at the prism vertices:

$$R_4^{[(4,6;0)p]}T_2^{[(0,6;0)p]}T_8^{[(2,4;0)p]}Al_2^{[(0,2;6)p]}Al_1^{[(0,4;4)p]}\times Al_{12}^{[(2,2;4)p]}Al_2^{[(0,0;10)p]}Al_2^{[(0,2;8)p]}Al_2^{[(0,4;6)p]} \quad (1)$$

or

$$R_x^{[(4,6)p]}T_y^{[(4x/y,6-4x/y)p]}Al_z, \quad (2)$$

taking into consideration that the pentagonal and trigonal prisms around the *R* and *T* atoms, respectively, are formed exclusively by the other two kinds of atom. The average composition of the trigonal prisms around the *T* atoms is $R_{1.6}Al_{4.4}$.

Another ten types from the list in Table 7 fulfill the condition that the prisms around *R* and *T* atoms are formed exclusively by other elements, however, the prisms have different compositions. The pentagonal prisms around the *R* atoms have the compositions Al_{10}, T_2Al_8, T_4Al_6, or T_6Al_4. The same composition of the pentagonal prism as for the $Ho_4Ni_{10}Ga_{21}$-type structure is observed only for the ZrNiAl-type structure. Consequently, the formulae (2) is valid also for the structure type ZrNiAl [19]. The average composition of the trigonal prisms (R_4Al_2) corresponds to one site centering an R_6 prism (multiplicity 2) and another site centering an Al_6 prism (multiplicity 1). The following formulas apply to the other nine structure types:

$$R_x^{[(0,10)p]}T_y^{[(0,6)p]}Al_z \quad (3)$$

for $CeFe_2Al_8$, $LaCoAl_4$ [20], and $UCoAl_4$ [21];

$$R_x^{[(2,8)p]}T_y^{[(2x/y,6-2x/y)p]}Al_z \quad (4)$$

for $Gd_3Ni_5Al_{19}$ [22], $Y_4Ni_6Al_{23}$ [23], $U_4Ni_5Al_{18}$ [24], $YNiAl_4$ [25], and $MgCuAl_2$ [26];

$$R_x^{[(6,4)p]}T_y^{[(6x/y,6-6x/y)p]}Al_z \quad (5)$$

for Mo_2FeB_2 [27].

Conclusions

The $Lu_4Ni_{10}Al_{21}$ compound is the first aluminide found to crystallize with a $Ho_4Ni_{10}Ga_{21}$-type structure. Isotypic compounds are known in rare-earth metal systems *R*–Ni–Ga and *R*–Pd–In.

The Lu atoms are situated at the centers of pentagonal prisms of composition Ni_4Al_6 and the Ni atoms center trigonal prisms of composition Al_6 and Lu_2Al_4, in the the ratio 1:4, which can be confirmed from the crystal-chemical formulae $R_x^{[(4,6)p]}T_y^{[(4x/y,6-4x/y)p]}Al_z$. The Al atoms center square and pentagonal prisms in a two-layer description.

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