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New quaternary compounds $R_2TAl_4Ge_2$ (R = Y, Sm, Gd-Lu, T = Fe, Ni)

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Nine rare-earth iron and nine rare-earth nickel alumogermanides $R_2FeAl_4Ge_2$ (R = Y, Sm, Gd, Tb, Dy, Ho, Er, Tm, Lu) and $R_2NiAl_4Ge_2$ (R = Y, Sm, Gd, Tb, Dy, Ho, Er, Tm, Yb) were synthesized by arc melting and their crystal structures were studied by X-ray powder diffraction. They are isotypic to $Tb_2NiAl_4Ge_2$, Pearson symbol *tI*18, space group *I*4/*mmm*. The tetragonal structure type $Tb_2NiAl_4Ge_2$ is a quaternary variant of the ternary type $Yb_3F_4S_2$: $Yb_3F_4S_2 \equiv (NiGe_2)Al_4Tb_2$. It belongs to a family of structures with cubic coordination of the smallest atoms (Fe or Ni).

Quaternary alumogermanide / X-ray powder diffraction / Crystal structure / Isotypic compounds

Introduction

The crystal structure of $Tb_2NiAl_4Ge_2$ (*tI*18, *I*4/*mmm*) was reported in [1]. Later, three isotypic compounds were observed in the Er–*T*–Al–Ge systems with T = Fe, Co, Ni [2,3]. The formation of a row of isotypic compounds $R_2CoAl_4Ge_2$ (R = Y, Sm, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu) was reported in [4], and in [5] two other rows of isotypic compounds $R_2FeAl_4Ge_2$ (R = Y, Sm, Gd, Tb, Dy, Ho, Er, Tm, Lu) and $R_2NiAl_4Ge_2$ (R = Y, Sm, Gd, Tb, Dy, Ho, Er, Tm, Yb) were observed. In total, today 27 quaternary compounds isotypic to $Tb_2NiAl_4Ge_2$ are known.

According to the Handbook of Inorganic Substances [6] and Pearson's Crystal Data [7], complete structure determinations have been performed for six compounds, $Gd_2TAl_4Ge_2$ (T = Fe, Co) [8], $Er_2TAl_4Ge_2$ (T = Fe, Co) [2,3], $Ho_2CoAl_4Ge_2$ [9], and $Tb_2NiAl_4Ge_2$ [1]. Cell parameters have been determined for another 12 compounds, $R_2FeAl_4Ge_2$ (R = Y, Tb, Dy, Ho) [8], $R_2CoAl_4Ge_2$ (R = Y, Sm, Tb, Dy, Tm, Yb, Lu) [8,9], and $Er_2NiAl_4Ge_2$ [2]. No crystallographic data are known for 10 other compounds. The crystal structure of the prototype was determined by X-ray single-crystal diffraction, whereas the crystal structures of the isotypic compounds were refined by X-ray powder diffraction.

The aim of the present work was to perform complete structure determinations for the quaternary compounds in the *R*–*T*–Al–Ge (R = Y, Sm, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu and T = Fe, Ni) systems adopting $Tb_2NiAl_4Ge_2$-type structures, the existence of which had been briefly reported in [5].

Experimental

Samples of nominal composition $R_{22.2}T_{11.1}Al_{44.5}Ge_{22.2}$ (R = Y, Sm, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu and T = Fe, Ni) were synthesized from the elements (purity of $R \geq 99.75$, $T \geq 99.99$, Al ≥ 99.998, Ge ≥ 99.999 mass%) by arc melting in a water-cooled copper crucible with a tungsten electrode under a purified argon atmosphere (using Ti as a getter). The ingots were annealed at 600°C under vacuum in quartz ampoules for 1 month and subsequently quenched in cold water. The weight loss during the preparation of the samples was less than 1 % of the total mass, which was 1 g for each alloy.

The crystal structures of the new compounds were established by X-ray powder diffraction. Data for polycrystalline samples were collected on an automatic diffractometer STOE Stadi P (Cu $K\alpha_1$ radiation, λ = 1.5406 Å) in the angular range $6 \leq 2\theta \leq 110.625°$ with a step of 0.015° and scan time 250 s. The structural parameters were refined by the Rietveld method [10], using the program DBWS [11]. The structure drawings were made with the program ATOMS [12].

Results and discussion

X-ray diffraction of the alloys showed that the samples $R_{22.2}Fe_{11.1}Al_{44.5}Ge_{22.2}$ with Y, Sm, Gd, Tb, Dy, Ho, Er, Tm, and Lu, as well as the samples $R_{22.2}Ni_{11.1}Al_{44.5}Ge_{22.2}$ with Y, Sm, Gd, Tb, Dy, Ho, Er, Tm, and Yb, contained the compounds $R_2FeAl_4Ge_2$ and $R_2NiAl_4Ge_2$, respectively. The crystal structures effectively belong to the $Tb_2NiAl_4Ge_2$ type. In addition to the new compounds $R_2TAl_4Ge_2$ (T = Fe, Ni), all the samples contained a small quantity (~ 3-5 mass%) of a secondary phase, RAlGe with YAlGe-type structure (*oS*12, *Cmcm*), or, in the case of the Sm-containing samples, a phase with α-$ThSi_2$-type structure (*tI*12, $I4_1/amd$). In the sample $Yb_{22.2}Ni_{11.1}Al_{44.5}Ge_{22.2}$ the secondary phase was $YbAl_2Ge_2$ with Ce_2SO_2-type structure (*hP*5, *P*-3*m*1).

The samples $Yb_{22.2}Fe_{11.1}Al_{44.5}Ge_{22.2}$ and $Lu_{22.2}Ni_{11.1}Al_{44.5}Ge_{22.2}$ did not contain the expected phases "$Yb_2FeAl_4Ge_2$" and "$Lu_2NiAl_4Ge_2$". In the sample with Yb the formation of the quaternary compound $Yb_3FeAl_3Ge_2$ with $Y_3NiAl_3Ge_2$-type structure (*hP*9, *P*-62*m*) was confirmed. The sample $Lu_{22.2}Ni_{11.1}Al_{44.5}Ge_{22.2}$ appeared to be multiphase with as dominant content the two ternary phases LuAlGe (YAlGe, *oS*12, *Cmcm*) and $LuNiAl_4$ ($YNiAl_4$, *oS*24, *Cmcm*). The cell parameters refined for the RAlGe compounds (R = Y, Sm, Gd, Tb, Dy, Ho, Er, Tm, Lu), $YbAl_2Ge_2$, $LuNiAl_4$, and $Yb_3FeAl_3Ge_2$ are in good agreement with those reported in the literature [7].

Based on the X-ray diffraction data, the structural parameters of the compounds $R_2FeAl_4Ge_2$ (R = Y, Sm, Gd, Tb, Dy, Ho, Er, Tm, Lu) and $R_2NiAl_4Ge_2$ (R = Y, Sm, Gd, Tb, Dy, Ho, Er, Tm, Yb) were determined.

Details of the structural refinements, refinable atomic coordinates and displacement parameters of the nine compounds $R_2FeAl_4Ge_2$ and nine compounds $R_2NiAl_4Ge_2$ are listed in Tables 1 and 3. The structure type $Tb_2NiAl_4Ge_2$ has a fully ordered atom arrangement, where each element occupies one site in space group *I*4/*mmm*. As expected, the cell parameters of the new compounds decrease with decreasing radius of the rare-earth metal [13] from Sm to Lu (Fig. 1). The parameters of the $R_2CoAl_4Ge_2$ compounds, shown in the same figure, are from [9]. For the three series, the cell parameters of the compounds with Yb do not fit into the general pattern, which can be explained by the valence state of Yb (II).

A comparison of the experimental and calculated diffraction diagrams for $Y_2FeAl_4Ge_2$ is shown in Fig. 2. Relevant interatomic distances for the new compounds are presented in Tables 2 and 4.

The structure of the compounds $R_2TAl_4Ge_2$ (T = Fe, Ni) belongs to the family of structures with cubic coordination of the smallest atoms (here the Fe or Ni atoms), which corresponds to class #8 of the classification by P. Krypyakevych [14]. The description of the coordination polyhedra is given on the example of $Y_2FeAl_4Ge_2$. The coordination polyhedron of the Fe atom consists exclusively of Al atoms, which form a cube (Al_8). The coordination polyhedron of the Ge atom is constructed from atoms of two kinds, Y and Al, and has the shape of a tetragonal antiprism of composition Y_4Al_4 with one additional Y atom above the square base formed by Y atoms. The Al atom is located at the center of a tetragonal prism of composition $Y_2Fe_2Al_4$ with three additional atoms – two Ge atoms above the side faces of composition Y_2Al_2 and one Al atom above the Fe_2 edge of the prism. The coordination polyhedron of the Y atom is a pentagonal prism of composition $Y_4Al_2Ge_4$ with four additional Y atoms above two of the rectangular faces and the two pentagonal bases, two Al atoms and one Ge atom above the three other rectangular faces, and one more Fe atom beyond the Al_2 edge of the prism. The content of one unit cell of the structure of $Y_2FeAl_4Ge_2$ and the coordination polyhedra of the different atoms are shown in Fig. 3.

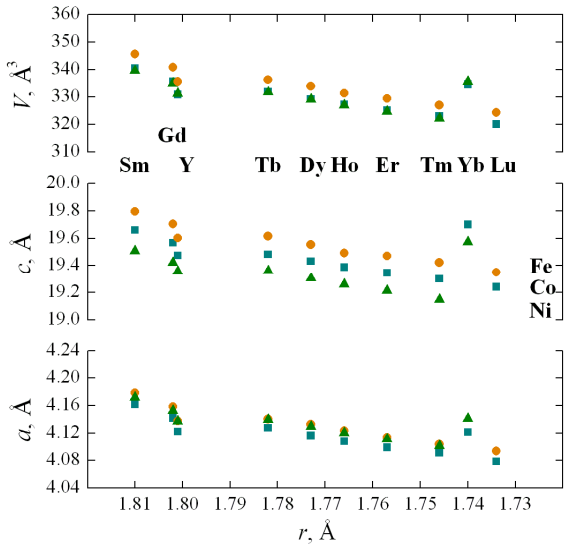

Fig. 1 Cell parameters of $R_2TAl_4Ge_2$ compounds.

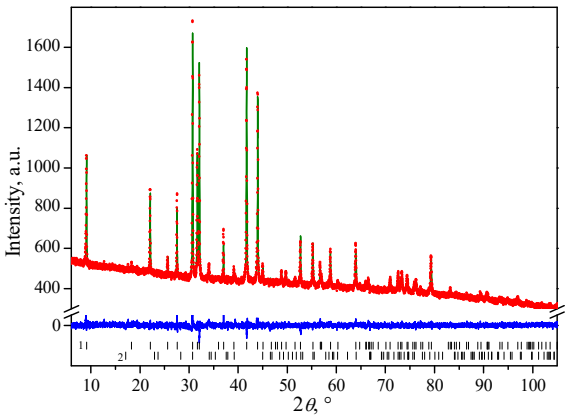

Fig. 2 Experimental, calculated and difference between experimental and calculated X-ray powder diffraction patterns (Cu $K\alpha_1$ radiation) for the sample $Y_{22.2}Fe_{11.1}Al_{44.5}Ge_{22.2}$. Vertical bars indicate the positions of the reflections of $Y_2FeAl_4Ge_2$ (1) and YAlGe (2).

Table 1 Details of the structural refinements of the compounds $R_2FeAl_4Ge_2$ (space group *I*4/*mmm*, *R* in 4*e*: 0 0 *z*, Fe in 2*a*: 0 0 0, Al in 8*g*: 0 ½ *z*, Ge in 4*e*: 0 0 *z*, *Z* = 2).

Compound		$Y_2FeAl_4Ge_2$	$Sm_2FeAl_4Ge_2$	$Gd_2FeAl_4Ge_2$	$Tb_2FeAl_4Ge_2$	$Dy_2FeAl_4Ge_2$	$Ho_2FeAl_4Ge_2$	$Er_2FeAl_4Ge_2$	$Tm_2FeAl_4Ge_2$	$Lu_2FeAl_4Ge_2$
Cell parameters, Å:	*a*	4.13752(2)	4.17774(5)	4.15214(4)	4.14087(5)	4.13081(6)	4.12275(3)	4.11352(7)	4.10381(6)	4.09686(5)
	c	19.6019(2)	19.7915(4)	19.6813(7)	19.6153(6)	19.5505(7)	19.4875(4)	19.4701(8)	19.4217(7)	19.3672(3)
Cell volume *V*, Å^3		335.57(3)	345.43(2)	339.31(3)	336.34(2)	333.60(3)	331.23(1)	329.45(3)	327.09(3)	325.06(2)
Density D_X, g cm^{-3}		4.8171	5.8608	6.1015	6.1912	6.3127	6.4044	6.4863	6.5681	6.7310
FWHM parameters:	*U*	0.057(3)	0.032(2)	0.073(3)	0.059(4)	0.061(3)	0.038(3)	0.055(2)	0.036(1)	0.031(1)
	V	-0.031(2)	-0.011(2)	-0.028(3)	-0.034(4)	-0.024(2)	-0.011(2)	-0.029(2)	-0.014(2)	-0.009(2)
	W	0.0108(5)	0.0097(6)	0.0088(5)	0.0117(6)	0.0148(5)	0.0085(7)	0.0101(4)	0.094(3)	0.0088(4)
Mixing parameter η		0.497(6)	0.554(7)	0.572(6)	0.631(7)	0.687(7)	0.746(6)	0.691(6)	0.595(4)	0.607(5)
Asymmetry parameter C_M		-0.063(6)	-0.067(7)	-0.054(8)	0.057(7)	0.081(6)	-0.081(7)	-0.072(6)	-0.081(7)	0.079(5)
Texture parameter *G*, direction [001]		0.891(2)	0.905(2)	0.897(1)	0.937(1)	0.914(2)	0.907(2)	0.984(1)	0.927(1)	0.934(1)
Atomic coordinates:	*z*(*R*)	0.18351(5)	0.18296(8)	0.18283(9)	0.18274(8)	0.18287(7)	0.18283(5)	0.18268(6)	0.18291(7)	0.18325(6)
	z(Al)	0.0656(2)	0.0653(3)	0.0664(4)	0.0646(4)	0.0656(3)	0.0659(2)	0.0647(4)	0.0658(3)	0.0666(3)
	z(Ge)	0.3351(2)	0.3375(2)	0.3371(3)	0.3375(4)	0.3368(2)	0.3343(1)	0.3334(3)	0.3362(3)	0.3338(2)
Isotropic	B_{iso}(*R*)	0.76(2)	0.87(4)	1.01(6)	0.95(5)	0.99(6)	1.28(3)	0.88(6)	0.97(5)	0.80(2)
displacement	B_{iso}(Fe)	0.74(5)	0.83(14)	1.12(11)	1.03(10)	1.09(13)	1.18(8)	0.95(14)	1.02(11)	1.01(9)
parameters, Å^2:	B_{iso}(Al)	1.14(3)	1.09(11)	1.46(14)	1.34(12)	1.14(11)	0.90(5)	1.18(15)	1.25(13)	1.15(10)
	B_{iso}(Ge)	0.88(3)	0.94(9)	1.09(13)	1.12(14)	1.11(13)	1.34(4)	0.97(13)	0.99(12)	1.08(9)
Reliability factors:	R_B	0.0551	0.0627	0.0487	0.0526	0.0591	0.0607	0.0607	0.0621	0.0532
	R_p	0.0222	0.0324	0.0115	0.0218	0.0273	0.0263	0.0241	0.0292	0.0263
	R_{wp}	0.0303	0.0381	0.0148	0.0284	0.0344	0.0358	0.0385	0.0318	0.0379

Table 2 Interatomic distances (δ, Å) in the compounds $R_2FeAl_4Ge_2$.

Compound	δ(Ge-4Al) δ(Al-2Ge)	δ(Ge-4*R*) δ(*R*-4Ge)	δ(Ge-1*R*) δ(*R*-1Ge)	δ(Al-2Fe) δ(Fe-8Al)	δ(Al-1Al)	δ(Al-4Al)	δ(Al-2*R*) δ(*R*-4Al)	δ(Fe-2*R*) δ(*R*-1Fe)	δ(*R*-4*R*)	δ(*R*-4*R*)
$Y_2FeAl_4Ge_2$	2.841(4)	2.9483(5)	2.972(4)	2.436(2)	2.572(6)	2.9257(1)	3.102(3)	3.5971(10)	3.9184(9)	4.13752(2)
$Sm_2FeAl_4Ge_2$	2.840(5)	2.9817(6)	3.059(4)	2.456(3)	2.585(8)	2.9541(1)	3.128(5)	3.6211(16)	3.9710(15)	4.17774(5)
$Gd_2FeAl_4Ge_2$	2.814(7)	2.9621(8)	3.036(6)	2.453(4)	2.614(11)	2.9360(1)	3.092(6)	3.5983(18)	3.9510(17)	4.15214(4)
$Tb_2FeAl_4Ge_2$	2.824(8)	2.9548(11)	3.036(8)	2.427(4)	2.534(11)	2.9280(1)	3.108(6)	3.5845(16)	3.9416(15)	4.14087(5)
$Dy_2FeAl_4Ge_2$	2.812(5)	2.9461(5)	3.009(4)	2.431(3)	2.565(8)	2.9209(1)	3.086(5)	3.5752(14)	3.9270(13)	4.13081(6)
$Ho_2FeAl_4Ge_2$	2.834(3)	2.9343(2)	2.952(2)	2.429(2)	2.569(6)	2.9152(1)	3.073(3)	3.5629(10)	3.9182(9)	4.12275(3)
$Er_2FeAl_4Ge_2$	2.858(7)	2.9255(6)	2.935(6)	2.412(4)	2.519(11)	2.9087(1)	3.083(6)	3.5568(12)	3.9157(11)	4.11352(7)
$Tm_2FeAl_4Ge_2$	2.799(6)	2.9255(8)	2.977(6)	2.417(3)	2.556(8)	2.9018(1)	3.063(4)	3.5524(14)	3.9002(13)	4.10381(6)
$Lu_2FeAl_4Ge_2$	2.814(5)	2.9157(5)	2.916(4)	2.421(3)	2.580(8)	2.8969(1)	3.050(4)	3.5490(12)	3.8829(11)	4.09686(5)

Table 3 Details of the structural refinements of the compounds $R_2NiAl_4Ge_2$ (space group *I*4/*mmm*, *R* in 4*e*: 0 0 *z*, Ni in 2*a*: 0 0 0, Al in 8*g*: 0 ½ *z*, Ge in 4*e*: 0 0 *z*, *Z* = 2).

Compound		$Y_2NiAl_4Ge_2$	$Sm_2NiAl_4Ge_2$	$Gd_2NiAl_4Ge_2$	$Tb_2NiAl_4Ge_2$	$Dy_2NiAl_4Ge_2$	$Ho_2NiAl_4Ge_2$	$Er_2NiAl_4Ge_2$	$Tm_2NiAl_4Ge_2$	$Yb_2NiAl_4Ge_2$
Cell parameters, Å:	*a*	4.13677(2)	4.17211(5)	4.15217(4)	4.13981(3)	4.12941(4)	4.12049(4)	4.11134(5)	4.10003(4)	4.14101(7)
	c	19.3558(3)	19.5064(7)	19.4187(5)	19.3622(4)	19.3054(5)	19.2608(6)	19.2134(6)	19.1809(6)	19.5732(8)
Cell volume *V*, Å^3		331.23(1)	339.54(4)	334.78(3)	331.83(3)	329.19(3)	327.02(4)	324.76(4)	322.43(4)	335.64(6)
Density D_X, g cm^{-3}		4.909	5.992	6.212	6.302	6.425	6.517	6.609	6.692	6.509
FWHM parameters:	*U*	0.048(2)	0.066(4)	0.087(3)	0.062(3)	0.049(1)	0.055(3)	0.071(3)	0.046(2)	0.094(3)
	V	-0.022(2)	-0.035(3)	-0.023(3)	-0.041(3)	-0.014(3)	-0.038(3)	-0.021(2)	-0.018(3)	-0.039(3)
	W	0.0098(4)	0.0101(6)	0.0092(4)	0.0106(5)	0.0120(4)	0.0099(6)	0.0117(5)	0.103(4)	0.0109(6)
Mixing parameter η		0.822(4)	0.774(5)	0.713(5)	0.776(4)	0.912(4)	0.705(6)	0.874(5)	0.911(6)	0.802(7)
Asymmetry parameter C_M		0.012(6)	0.015(8)	-0.053(4)	-0.039(4)	0.010(5)	-0.035(7)	0.009(6)	-0.038(6)	0.022(7)
Texture parameter *G*, direction [001]		0.956(1)	0.961(2)	1.028(2)	0.979(1)	0.983(1)	0.985(2)	1.007(2)	1.003(1)	0.886(2)
Atomic coordinates:	*z*(*R*)	0.18579(6)	0.18562(8)	0.18581(6)	0.18558(7)	0.18544(6)	0.18527(7)	0.18546(8)	0.18573(7)	0.18561(8)
	z(Al)	0.0699(3)	0.0683(5)	0.0675(3)	0.0687(5)	0.0669(4)	0.0678(6)	0.0653(6)	0.0658(5)	0.0642(7)
	z(Ge)	0.3394(2)	0.3403(4)	0.3382(2)	0.3405(4)	0.3402(3)	0.3399(4)	0.3389(5)	0.3387(4)	0.3408(5)
Isotropic	B_{iso}(*R*)	0.98(2)	1.06(6)	1.09(8)	0.92(6)	0.97(8)	1.08(7)	0.99(7)	0.95(9)	1.12(9)
displacement	B_{iso}(Ni)	0.96(4)	1.05(12)	1.22(12)	0.99(12)	1.14(12)	1.19(9)	1.05(11)	0.99(12)	1.08(11)
parameters, Å^2:	B_{iso}(Al)	1.22(4)	1.38(13)	1.41(13)	1.26(14)	1.18(12)	1.28(11)	1.16(13)	1.18(14)	1.28(14)
	B_{iso}(Ge)	1.12(2)	1.18(8)	1.15(14)	1.09(13)	1.07(11)	1.14(10)	1.03(12)	1.06(13)	1.15(12)
Reliability factors:	R_B	0.0462	0.0755	0.0479	0.0486	0.0524	0.0576	0.0588	0.0543	0.0641
	R_p	0.0201	0.0485	0.0316	0.0347	0.0337	0.0443	0.0389	0.0352	0.0457
	R_{wp}	0.0287	0.0421	0.0263	0.0262	0.0291	0.0371	0.0306	0.0299	0.0334

Table 4 Interatomic distances (δ, Å) in the compounds $R_2NiAl_4Ge_2$.

Compound	δ(Ge-4Al) δ(Al-2Ge)	δ(Ge-4*R*) δ(*R*-4Ge)	δ(Ge-1*R*) δ(*R*-1Ge)	δ(Al-2Ni) δ(Ni-8Al)	δ(Al-1Al)	δ(Al-4Al)	δ(Al-2*R*) δ(*R*-4Al)	δ(Ni-2*R*) δ(*R*-1Ni)	δ(*R*-4*R*)	δ(*R*-4*R*)
$Y_2NiAl_4Ge_2$	2.713(5)	2.9655(7)	2.973(4)	2.472(3)	2.706(8)	2.9251(1)	3.051(4)	3.5961(12)	3.8386(11)	4.13677(2)
$Sm_2NiAl_4Ge_2$	2.744(8)	2.9931(13)	3.017(8)	2.475(5)	2.665(14)	2.9501(1)	3.097(7)	3.6208(16)	3.8745(14)	4.17211(5)
$Gd_2NiAl_4Ge_2$	2.768(5)	2.9728(6)	2.959(4)	2.455(3)	2.622(8)	2.9362(1)	3.097(4)	3.6082(12)	3.8516(11)	4.15217(4)
$Tb_2NiAl_4Ge_2$	2.716(8)	2.9705(13)	3.000(8)	2.461(5)	2.660(14)	2.9273(1)	3.067(7)	3.5932(14)	3.8461(12)	4.13981(3)
$Dy_2NiAl_4Ge_2$	2.735(6)	2.9616(10)	2.988(6)	2.435(4)	2.583(11)	2.9199(1)	3.082(6)	3.5800(12)	3.8392(11)	4.12941(4)
$Ho_2NiAl_4Ge_2$	2.721(9)	2.9537(13)	2.978(8)	2.439(6)	2.612(16)	2.9136(1)	3.060(9)	3.5684(14)	3.8349(12)	4.12049(4)
$Er_2NiAl_4Ge_2$	2.759(10)	2.9446(15)	2.948(10)	2.408(6)	2.509(16)	2.9072(1)	3.091(9)	3.5633(15)	3.8213(14)	4.11134(5)
$Tm_2NiAl_4Ge_2$	2.749(8)	2.9368(12)	2.934(8)	2.407(5)	2.524(14)	2.8992(1)	3.081(7)	3.5625(13)	3.8058(12)	4.10003(4)
$Yb_2NiAl_4Ge_2$	2.783(11)	2.9734(17)	3.038(10)	2.422(7)	2.513(19)	2.9281(1)	3.152(10)	3.6330(16)	3.8636(14)	4.14101(7)

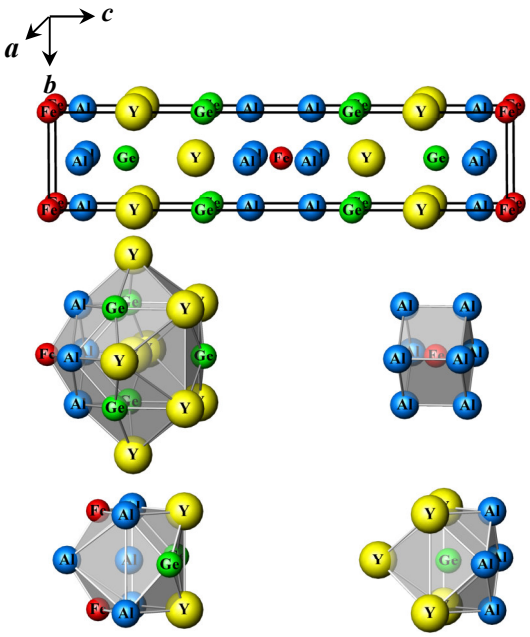

Fig. 3 Unit-cell content of the structure of the $Y_2FeAl_4Ge_2$ compound and coordination polyhedra of the atoms.

The structure of the $Tb_2NiAl_4Ge_2$ type can be considered as an alternation of two types of layer containing cubes along the crystallographic direction [001]. The first type of layer is formed by cubes of composition Al_8, every second cube being centered by a Ni atom, while the second type of layer is formed by slightly distorted empty cubes of composition Tb_4Ge_4. The formula of the compound can be written as $NiAl_4 + Tb_2Ge_2 \equiv Tb_2NiAl_4Ge_2$. The arrangement of cubes in the structure of $Y_2FeAl_4Ge_2$ is shown in Fig. 4. The quaternary structure type $Tb_2NiAl_4Ge_2$ is an ordering variant of the ternary type $Yb_3F_4S_2$ [15] (antitype), $[NiGe_2]Al_4Tb_2$ [16].

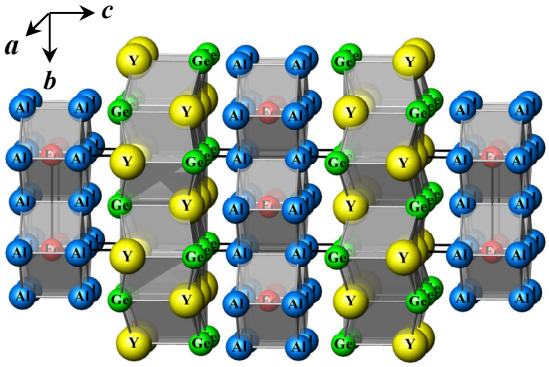

Fig. 4 Alternation of two types of layer containing cubes along the crystallographic direction [001] in the structure of $Y_2FeAl_4Ge_2$.

Conclusions

The quaternary compounds $R_2FeAl_4Ge_2$ (R = Y, Sm, Gd, Tb, Dy, Ho, Er, Tm, Lu) and $R_2NiAl_4Ge_2$ (R = Y, Sm, Gd, Tb, Dy, Ho, Er, Tm, Yb) adopt the structure type $Tb_2NiAl_4Ge_2$, which belongs to a family of structures with cubic coordination of the small atoms (Fe/Ni). Their structure can be described as a packing of monocapped square antiprisms $[GeAl_4R_5]$ and cubes $[TAl_8]$ (T = Fe, Ni).

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