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Crystal structure of the compound $Tb_{0.67}Pt_2Al_5$

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The crystal structure of the ternary compound $Tb_{0.67}PtAl_5$ (structure type $Sc_{0.6}Fe_2Si_{4.9}$, *hP*20-4.67, $P6_3/mmc$, *a* = 4.2734(10), *c* = 16.391(3) Å) was refined from X-ray single-crystal diffraction data. It contains two kinds of slab stacked along [0 0 1]: slightly puckered layers of composition $PtAl_2$ and flat layers $Tb_{0.67}Al$ with disordered distribution of Tb atoms and Al_3 triangles. Using group-subgroup relations, a hypothetical structure $R_2T_6Al_{15}$ with fully ordered distribution of *R* atoms and Al_3 triangles was derived (*oS*92, *Cmcm*, *a* = 12.820, *b* = 7.4017, *c* = 16.391 Å). Both structures together with some other structure types of ternary aluminides belong to a homologous series with the general formula $R_{0.67}T_nM_{2n+1}$.

Aluminide / Terbium / Platinum / Single-crystal X-ray diffraction / Crystal-chemical analysis

Introduction

Three ternary compounds have been reported up to date in the system Tb-Pt-Al: $Tb_{0.67}Pt_2Al_5$ (structure type $Sc_{0.6}Fe_2Si_{4.9}$, space group $P6_3/mmc$, *a* = 4.278, *c* = 16.408 Å [1]), $Tb_4Pt_9Al_{24}$ (structure type $Er_4Pt_9Al_{24}$, space group $P\bar{1}$, *a* = 7.494, *b* = 7.494, *c* = 13.104 Å, α = 84.53, β = 79.01, γ = 60.0° [2]), and TbPtAl (structure type TiNiSi, space group *Pnma*, *a* = 6.921, *b* = 4.396, *c* = 7.967 Å [3]). The solid solutions based on the binary compounds $TbPt_2$ and $TbAl_2$ with $MgCu_2$-type structure (space group $Fd\bar{3}m$) were investigated in [3]: $TbPt_{2-1.8}Al_{0-0.2}$ (*a* = 7.612-7.615 Å) and $TbPt_{0-0.5}Al_{2-1.5}$ (*a* = 7.865-7.771 Å). For the compound $Tb_{0.67}Pt_2Al_5$ [1] cell parameters were determined and structure type assigned, however, the atomic coordinates were not refined. The structure type $Sc_{0.67}Fe_2Si_{4.9}$ [4] has representatives among aluminides, gallides, silicides, and germanides [5]: ternary $Zr_{0.5}Pt_2Al_{5.11}$ [1], $R_{0.67}Pt_2Al_5$ (*R* = Y, Ce, Gd-Tm) [1,6,7], $Ce_{0.67}Pt_2Ga_5$ [8], $R_{0.6}Fe_2Si_{4.9}$ (*R* = Sc, Y, Gd-Lu) [4,9,10], and quaternary $Gd_{0.67}Pt_2Al_4Si$ [6], $Y_{0.59}Ni_2Ga_{4.40}Ge_{0.60}$, $Sm_{0.53}Ni_2Ga_{4.56}Ge_{0.44}$, $Tb_{0.67}Ni_2Ga_{4.76}Ge_{0.24}$, $Ho_{0.67}Ni_2Ga_{4.4}Ge_{0.6}$ [11].

The structure type $Sc_{0.6}Fe_2Si_{4.9}$ is characterized by the presence of layers containing Sc atoms and Si_3 triangles. This and some other structure types, such as $DyNi_3Al_9$, $ErNi_3Al_9$ [12], $Gd_{1.33}Pt_3Al_8$ [6], $Er_{1.33}Pt_3Al_8$, $Y_4Pt_9Al_{24}$, $Er_4Pt_9Al_{24}$ [2], $Tb_{0.67}PdAl_3$ [13], $Ho_2Rh_3Al_9$ [14], and $Y_2Co_3Ga_9$ [15], forming in *R*-*T*-Al ternary systems (where *R* is a rare-earth metal and *T* a *d*-element of group VIII), are members of a homologous series [13]. The structures of this series are built up from slabs with a close-packed motif, but differ by the ratio of different slabs and the degree of ordering of *R* atoms and M_3 triangles.

The aim of the present work was to perform a detailed crystal-chemical analysis of the compound $Tb_{0.67}Pt_2Al_5$ based on crystallographic data determined from X-ray single-crystal diffraction.

Experimental

An alloy of nominal composition $Tb_{11}Pt_{24}Al_{65}$ was synthesized from the elements (Tb ≥ 99.83 wt.%, Pt ≥ 99.9 wt.%, 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. The ingot was annealed at 600°C in a quartz ampoule under vacuum for one month and subsequently quenched in cold water. The weight loss during the preparation of the sample was 0.4 % of the total mass, which was 1.2 g.

A prism-like single crystal was extracted from the alloy, mounted on a glass fiber and X-ray diffraction data were collected in the ω-2θ scan mode at room temperature on a CAD-4T diffractometer (Mo *K*α radiation, λ = 0.71073 Å). An analytical absorption correction was applied. No significant variation of the intensities was observed during the data collection. Hexagonal symmetry and the cell parameters *a* = 4.2734(10), *c* = 16.391(3) Å, obtained by a least-squares refinement of the angles of 25 reflections,

Table 1 Experimental details of the structure investigation and crystallographic data for the compound $Tb_{0.67}Pt_2Al_5$.

Structure type		$Sc_{0.6}Fe_2Si_{4.9}$
Pearson symbol		*hP*20-4.67
Space group		$P6_3/mmc$ (#194)
Formula units per cell *Z*		2
Cell parameters:	*a*, Å	4.2734(10)
	c, Å	16.391(3)
Cell volume *V*, Å^3		259.23(10)
Formula weight M_r		631.57
Density D_x, g cm^{-3}		8.091
Absorption coefficient μ, mm^{-1}		63.507
Crystal size, mm		0.035 × 0.035 × 0.055
Number of reflections:	measured	565
	independent	152
	with $I > 2\sigma(I)$	106
Reliability factor R_{int}		0.0455
Range of *h*, *k*, *l*		$0 \le h \le 5$, $0 \le k \le 5$, $-22 \le l \le 22$
Range θ, °		2.49-30.43
Reliability factors:	*R* (all)	0.0322
	R ($I > 2\sigma(I)$)	0.0308
	wR (all)	0.0491
	wR ($I > 2\sigma(I)$)	0.0488
	S	0.673
Number of reflections used in refinement		152
Number of refined parameters		17
Weighting scheme ($P = (F_o^2 + 2F_c^2)/3$)		$w = 1/[(\sigma F_o)^2 + (0.01P)^2]$
Residual electron density:	$\Delta\rho_{max}$, e Å^{-3}	2.290
	$\Delta\rho_{min}$, e Å^{-3}	-1.466
Extinction coefficient		0.0087(12)

Table 2 Atom coordinates, site occupancies, and displacement parameters (Å^2) for the structure of the compound $Tb_{0.67}Pt_2Al_5$ (structure type $Sc_{0.6}Fe_2Si_{4.9}$, *hP*20-4.67, $P6_3/mmc$, *a* = 4.2734(10), *c* = 16.391(3) Å).

Site	Wyckoff position	*x*	*y*	*z*	U_{eq}	Occupancy
Tb	2*c*	⅓	⅔	¼	0.0065(5)	0.67
Pt	4*f*	⅓	⅔	0.60878(7)	0.0056(3)	1
Al1	6*h*	0.546(3)	0.092(6)	¼	0.011(4)	0.33
Al2	4*f*	⅓	⅔	0.0472(4)	0.0074(15)	1
Al3	4*e*	0	0	0.1357(5)	0.0079(15)	1

Site	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Tb	0.0049(7)	0.0049(7)	0.0098(12)	0.0025(4)	0	0
Pt	0.0053(4)	0.0053(4)	0.0061(5)	0.00265(18)	0	0
Al1	0.016(8)	0.009(8)	0.005(4)	0.004(4)	0	0
Al2	0.008(2)	0.008(2)	0.004(3)	0.0041(11)	0	0
Al3	0.006(2)	0.006(2)	0.011(3)	0.0032(11)	0	0

indicated a $Sc_{0.6}Fe_2Si_{4.9}$-type structure (space group $P6_3/mmc$). A full-matrix least-squares refinement of the positional and anisotropic displacement parameters for the $Tb_{0.67}Pt_2Al_5$ compound was performed on F^2 using the SHELXL-97 program [16]. The atomic coordinates reported for $Y_{0.67}Pt_2Al_5$ in [1] were used as starting model. Trial refinements in the noncentrosymmetric space groups $P6_3mc$ and $P\bar{6}2c$ did not improve the results. Crystal data and details of the data collection and structure refinement for $Tb_{0.67}Pt_2Al_5$ are given in Table 1.

Results and discussion

The least-squares refinement confirmed the classification of the $Tb_{0.67}Pt_2Al_5$ structure into the $Sc_{0.6}Fe_2Si_{4.9}$ type. The refined atom coordinates and displacement parameters are listed in Table 2. As can be seen, a statistical disorder of single Tb atoms (Wyckoff position 2*c*) and groups of three Al atoms forming triangles (Wyckoff position 6*h*) is observed in the layers at *z* = ¼ and ¾. The occupancy of the site in Wyckoff position 6*h* cannot exceed one third because

Table 3 Interatomic distances (δ) and coordination numbers (CN) for the structure of the compound $Tb_{0.67}Pt_2Al_5$.

Atoms		δ, Å	CN
Tb[a]	– 3 Al1[b]	3.013(15)	20
	– 6 Al3	3.098(5)	
	– 2 Al2	3.324(6)	
	– 6 Pt	3.3831(9)	
	– 3 Tb[a]	4.2734(10)	
Pt	– 1 Al1[b]	2.480(8)	10
	– 3 Al3	2.5064(15)	
	– 1 Al2	2.557(6)	
	– 3 Al2	2.666(2)	
	– 2 Tb[a]	3.3831(9)	
Al1[b]	– 2 Pt	2.480(8)	10
	– 2 Al1[b]	2.73(4)	
	– 4 Al3	2.862(6)	
	– 2 Tb[a]	3.013(15)	
Al2	– 1 Pt	2.557(6)	11
	– 3 Pt	2.666(2)	
	– 3 Al3	2.862(5)	
	– 3 Al2	2.912(6)	
	– 1 Tb[a]	3.324(6)	
Al3	– 3 Pt	2.5064(15)	10
	– 3 Al2	2.862(5)	
	– 2 Al1[b]	2.862(6)	
	– 2 Tb[a]	3.098(5)	

[a] occ. (Tb) = 0.67; [b] occ. (Al1) = 0.33

Table 4 Transformation from the disordered structure of the compound $Tb_{0.67}Pt_2Al_5$ ($Sc_{0.6}Fe_2Si_{4.9}$ type) to the ordered hypothetical structure $R_2T_6Al_{15}$.

Model	**I** ($Tb_{0.67}Pt_2Al_5$)	**II**	**III** ($R_2T_6Al_{15}$)
Transformation matrix		$\begin{matrix}2 & 1 & 0\\ -1 & 1 & 0\\ 0 & 0 & 1\end{matrix}$	$\begin{matrix}3 & 3 & 0\\ -1 & 1 & 0\\ 0 & 0 & 1\end{matrix}$
Space group	(194) $P6_3/mmc$	(193) $P6_3/mcm$	(63) $Cmcm$
Cell parameters, Å	$a_I = 4.2734$ ($b_I = a_I = 4.2734$) $c_I = 16.391$	$a_{II} = \sqrt{3}\, a_I = 7.4017$ ($b_{II} = \sqrt{3}\, a_I = 7.4017$) $c_{II} = c_I = 16.391$	$a_{III} = 3a_I = 12.820$ $b_{III} = \sqrt{3}\, a_I = 7.4017$ $c_{III} = c_I = 16.391$
Site, Wyckoff position, coordinates	Tb 2*c* ⅓,⅔,¼	*R* 6*g* 0.3333,0,¼	*R*1 8*g* 0.3333,0.3333,¼
			*R*2 4*c* 0,0.3333,¼
	Pt 4*f* ⅓,⅔,0.6088	*T* 12*k* 0.6667,0,0.1088	*T*1 16*h* 0.1667,0.1667,0.1088
			*T*2 6*f* 0,0.6667,0.1088
	Al1 6*h* 0.546,0.092,¼	Al1 12*j* 0.213,0.333,¼	Al1 8*g* 0.106,0.227,¼
			Al2 8*g* 0.167,0.046,¼
			Al3 8*g* 0.440,0.227,¼
		Al2 6*g* 0.546,0,¼	Al4 8*g* 0.227,0.227,¼
			Al5 4*c* 0,0.546,¼
	Al2 4*f* ⅓,⅔,0.0472	Al3 12*k* 0.3333,0,0.0472	Al6 16*h* 0.3333,0.3333,0.0472
			Al7 8*f* 0,0.3333,0.0472
	Al3 4*e* 0,0,0.1357	Al4 8*h* ⅓,⅔,0.1357	Al8 16*h* 0.1667,0.5000,0.1357
		Al5 4*e* 0,0,0.1357	Al9 8*f* 0,0.0000,0.1357
Origin shift[a]	0,0,0	0,0,½	0,0,½

[a] The atom coordinates were standardized by the program STRUCTURE TIDY [17].

Table 5 Atom coordinates for the hypothetical structure $R_2T_6Al_{15}$ (*oS*92, *Cmcm*, a = 12.820, b = 7.4017, c = 16.391 Å).

Site	Wyckoff position	x	y	z
R	8*g*	0.1667	0.1667	¼
$T1$	16*h*	0.3333	0.3333	0.1088
$T2$	8*f*	0	0.3333	0.1088
Al1	16*h*	0.1667	0.1667	0.0472
Al2	16*h*	0.3333	0.0000	0.1357
Al3	8*g*	0.3940	0.2730	¼
Al4	8*f*	0	0.0000	0.1357
Al5	8*f*	0	0.3333	0.5472
Al6	4*c*	0	0.4540	¼

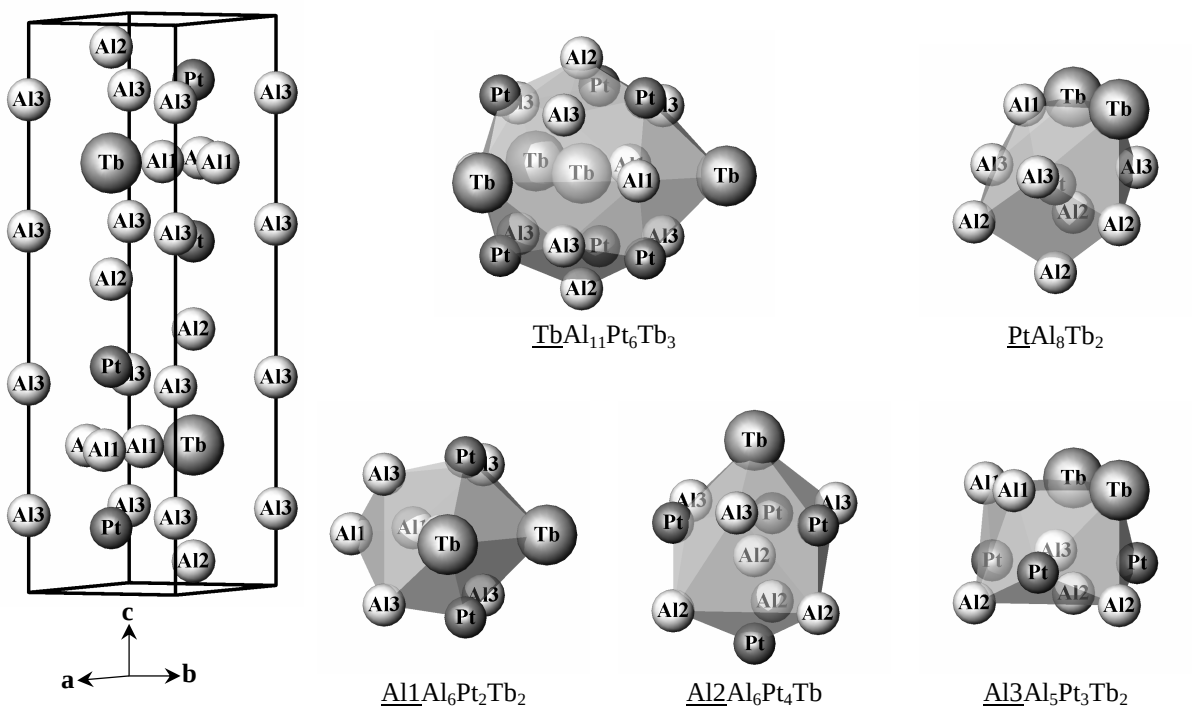

Fig. 1 Content of the unit cell and coordination polyhedra of the atoms in the structure of the compound $Tb_{0.67}Pt_2Al_5$.

higher occupancy would lead to the appearance of impossibly short Al-Al distances (1.54 Å) in the structure. On the contrary, the site in Wyckoff position 2*c* can be fully occupied by Tb atoms, if occ. (6*h*) = 0. During the preliminary structure refinement, the occupancies of the Wyckoff positions 6*h* and 2*c* were allowed to vary. It led to a refined ratio of rare-earth-metal atoms to Al_3 triangles close to the ideal value 2:1 (occ.(2*c*) = 0.69(1), occ.(6*h*) = 0.30(1)). Therefore, in the final refinement the occupancy of the Tb site in Wyckoff position 2*c* was fixed at the value 0.67, and the occupancy of the Al site in 6*h* at 0.33.

The content of the unit cell and the coordination polyhedra for the five independent atom positions in the $Tb_{0.67}Pt_2Al_5$ structure are shown in Fig. 1, and the interatomic distances within the coordination polyhedra are listed in Table 3. The Tb atoms center 20-vertex polyhedra $\underline{Tb}Al_{11}Pt_6Tb_3$, which can be described as deformed hexagonal prisms of composition Al_6Pt_6 with three Tb and five additional Al atoms capping the eight faces. The coordination polyhedra around the Pt and Al atoms are derivatives of an icosahedron with one or two missing vertices: $\underline{Pt}Al_8Tb_2$, $\underline{Al1}Al_6Pt_2Tb_2$, $\underline{Al2}Al_6Pt_4Tb$, and $\underline{Al3}Al_5Pt_3Tb_2$. These polyhedra are very similar to those observed in structure types of other aluminides containing layers with disordered or ordered distribution of rare-earth-metal atoms and Al_3 triangles ($Tb_{0.67}PdAl_3$, $Ho_2Rh_3Al_9$, $Y_2Co_3Ga_9$, $Gd_{1.33}Pt_3Al_8$, $Er_{1.33}Pt_3Al_8$, $Y_4Pt_9Al_{24}$, $Er_4Pt_9Al_{24}$, $R_{0.67}Ni_2Al_6$ (hypothetical) [12], $DyNi_3Al_9$, and $ErNi_3Al_9$) [13]. In the structure of $Tb_{0.67}Pt_2Al_5$ the

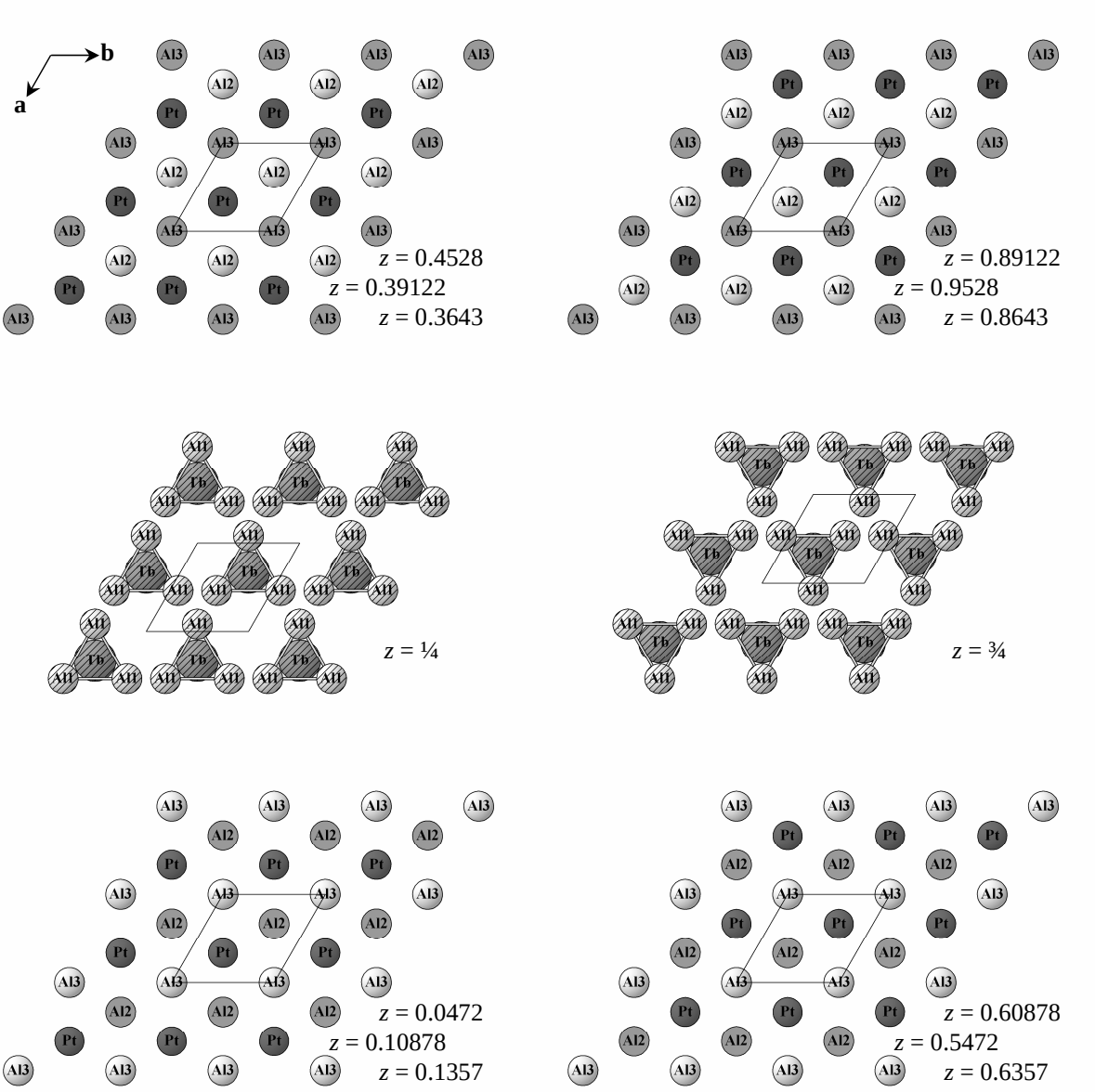

Fig. 2 $Tb_{0.67}Al$ and $PtAl_2$ slabs in the structure of the compound $Tb_{0.67}Pt_2Al_5$.

distances between the Al atoms forming triangles (2.73(4) Å) are shorter than the other Al-Al interatomic distances (2.862(6)-2.912(6) Å) indicating strong interaction. The shortest contact distances in the structure are observed between the Al atoms forming triangles and Pt atoms (2.480(8) Å).

The structure of $Tb_{0.67}Pt_2Al_5$ is built up from two kinds of slab, stacked along [0 0 1]. As can be seen from Fig. 2, one of them (a puckered slab of thickness 1.451 Å), of composition $PtAl_2$, is formed by Al and Pt layers possessing the motif of close-packed layers with triangular mesh (a Pt monoatomic layer is situated between two Al-atom layers; the Pt-Al interatomic distances are 2.5064(15) and 2.666(2) Å). In the second kind of slab (flat layer), of composition $Tb_{0.67}Al$ (Tb_2Al_3), the Tb atoms and the centers of the Al_3 triangles also form a triangular mesh. These slabs derive from close-packed *R*-atom layers by the replacement of one third of the Tb atoms by Al_3 triangles. The unit cell of $Tb_{0.67}Pt_2Al_5$ contains six slabs: two $Tb_{0.67}Al$ and four $PtAl_2$ in the sequence $PtAl_2$-$Tb_{0.67}Al$-$PtAl_2$-$PtAl_2$-$Tb_{0.67}Al$-$PtAl_2$.

In the $Tb_{0.67}Al$ layers the Tb atoms and the centers of the Al_3 triangles have the coordinates $x = ⅓$, $y = ⅔$ at $z = ¼$ and $x = ⅔$, $y = ⅓$ at $z = ¾$ (see Fig. 2). The atom arrangement within the layers is probably ordered and the observed disorder due to stacking faults with the probability 2:1 to find a Tb atom or an Al_3 triangle at the mentioned positions. For the members of the homologous series $R_{0.67}T_nM_{2n+1}$ (structure types $Tb_{0.67}PdAl_3$, $Ho_2Rh_3Al_9$, $Y_2Co_3Ga_9$, $Sc_{0.6}Fe_2Si_{4.9}$, $Gd_{1.33}Pt_3Al_8$, $Er_{1.33}Pt_3Al_8$, $Y_4Pt_9Al_{24}$,

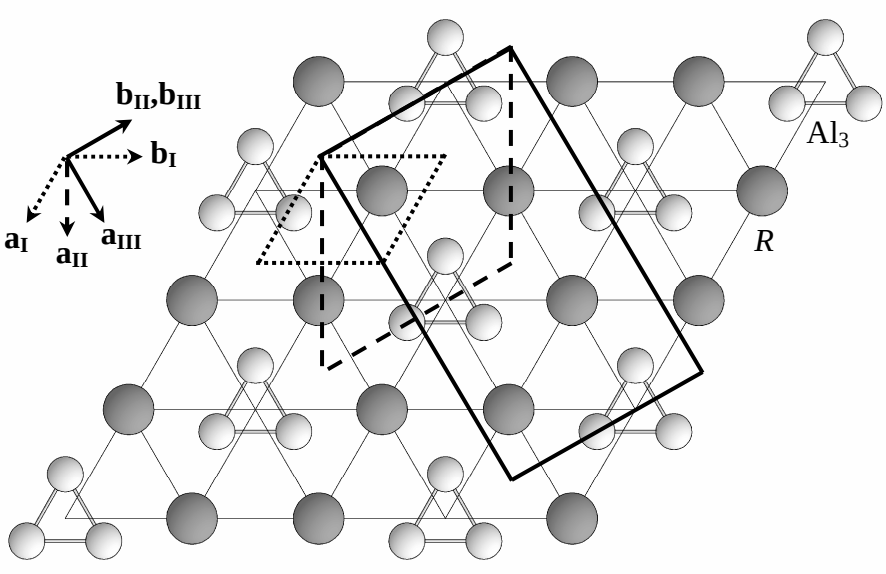

Fig. 3 Relation between the unit cells of $Tb_{0.67}Pt_2Al_5$ ($Sc_{0.6}Fe_2Si_{4.9}$ type) and hypothetical $R_2T_6Al_{15}$ showing only one $R_{0.67}M$ layer.

$Er_4Pt_9Al_{24}$) the M_3 triangles within a $R_{0.67}M$ layer have always the same orientation. When the layers are stacked, the M_3 triangles in "consecutive" $R_{0.67}M$ layers are oriented alternatively "up" and "down".

So far, only $R_{0.67}T_nM_{2n+1}$ structures with n = 1, 1.5, and 2 have been reported. Hexagonal $Tb_{0.67}PdAl_3$ (space group $P6_3/mmc$) with n = 1 contains four slabs in the unit cell along the crystallographic direction [0 0 1]: $PdAl_2$-$Tb_{0.67}Al$-$PdAl_2$-$Tb_{0.67}Al$. The *R* atoms and M_3 triangles are statistically disordered. Orthorhombic $Ho_2Rh_3Al_9$ and $Y_2Co_3Ga_9$ (*Cmcm*) are partly and fully ordered derivatives of $Tb_{0.67}PdAl_3$, respectively. Ordered derivatives of the $Sc_{0.6}Fe_2Si_{4.9}$ type with n = 2 have not yet been reported. The unit cell of rhombohedral $Gd_{1.33}Pt_3Al_8$ ($R\bar{3}m$) with n = 1.5, which is an intergrowth of $Tb_{0.67}PdAl_3$- and $Sc_{0.67}Fe_2Si_5$-type slabs in the ratio 1:1, contains 15 slabs: $PtAl_2$-$Gd_{0.67}Al$-$PtAl_2$-$PtAl_2$-$Gd_{0.67}Al$-$PtAl_2$-$Gd_{0.67}Al$-$PtAl_2$-$PtAl_2$-$Gd_{0.67}Al$-$PtAl_2$-$Gd_{0.67}Al$-$PtAl_2$-$PtAl_2$-$Gd_{0.67}Al$. Monoclinic $Er_{1.33}Pt_3Al_8$ (*C*2/*m*) and triclinic $Y_4Pt_9Al_{24}$ ($P\bar{1}$) are partly ordered variants of $Gd_{1.33}Pt_3Al_8$, whereas triclinic $Er_4Pt_9Al_{24}$ ($P\bar{1}$) is characterized by complete ordering of *R* atoms and Al_3 triangles. The last three structures contain five slabs along the stacking direction: $PtAl_2$-$R_{0.67}Al$-$PtAl_2$-$PtAl_2$-$R_{0.67}Al$. Other simple members of the homologous series $R_{0.67}T_nM_{2n+1}$ should have n = 1.33 (three $R_{0.67}M$ layers for four TM_2 slabs) and n = 1.67 (three $R_{0.67}M$ layers for five TM_2 slabs).

An ordered variant of the $Sc_{0.6}Fe_2Si_{4.9}$ type was derived. As can be seen from Table 4, the symmetry of the hypothetical structure $R_2T_6Al_{15}$ is orthorhombic, space group *Cmcm*, and the cell parameter *c* is the same as that of $Tb_{0.67}Pt_2Al_5$ (six slabs stacked along [0 0 1]). The orthorhombic cell of $R_2T_6Al_{15}$ is derived by tripling the hexagonal cell of $Tb_{0.67}Pt_2Al_5$ in the (0 0 1) plane and considering the orthohexagonal cell (Fig. 3). The resulting unit cell has six times larger volume. The group-subgroup relation for the corresponding space groups is the following:

$P6_3/mmc$ ($\mathbf{a_I}$, $\mathbf{b_I}$, $\mathbf{c_I}$) $\xrightarrow{\text{IIb}}$ $P6_3/mcm$ ($\mathbf{a_{II}} = 2\mathbf{a_I} + \mathbf{b_I}$, $\mathbf{b_{II}} = -\mathbf{a_I} + \mathbf{b_I}$, $\mathbf{c_{II}} = \mathbf{c_I}$) $\xrightarrow{\text{I}}$ *Cmcm* ($\mathbf{a_{III}} = 2\mathbf{a_{II}} + \mathbf{b_{II}}$, $\mathbf{b_{III}} = \mathbf{b_{II}}$, $\mathbf{c_{III}} = \mathbf{c_{II}}$) [18].

Ordering of *R* atoms and Al_3 triangles is not possible in the intermediate superstructure **II** with space group $P6_3/mcm$, since only one Wyckoff position is available for the rare-earth-metal atoms (6*g*) and the Al atoms in the Wyckoff position 6*g* do not form triangles. On the contrary, in the orthorhombic structure two sites are available for *R* atoms and five positions for Al atoms forming triangles. Completely ordered distribution of *R* atoms and Al_3 triangles is achieved when the Wyckoff position 4*c* (site *R*2) and three positions 8*g* (Al2, Al3 and Al4) are vacant. The atom coordinates for the hypothetical structure $R_2T_6Al_{15}$ with 92 atoms in the cell are listed in Table 5. The content of the unit cell and the coordination polyhedra of the nine independent atom positions are shown in Fig. 4. The latter are analogous to the polyhedra observed in the structure of the compound $Tb_{0.67}Pt_2Al_5$.

The structure types $R_{0.67}Ni_2Al_6$ (hypothetical), $DyNi_3Al_9$, and $ErNi_3Al_9$ are closely related to the structures of the homologous series $R_{0.67}T_nM_{2n+1}$. Like $Tb_{0.67}Pt_2Al_5$ ($Sc_{0.6}Fe_2Si_{4.9}$ type) and $R_2T_6Al_{15}$ (hypothetical) they contain $R_{0.67}M$ and TM_2 slabs stacked in ratio 1:2, however, consecutive TM_2 slabs are separated by an additional monoatomic layer formed by *M* atoms and all M_3 triangles have the same orientation. The stacking sequence of the slabs in the translation unit of the hypothetical hexagonal structure

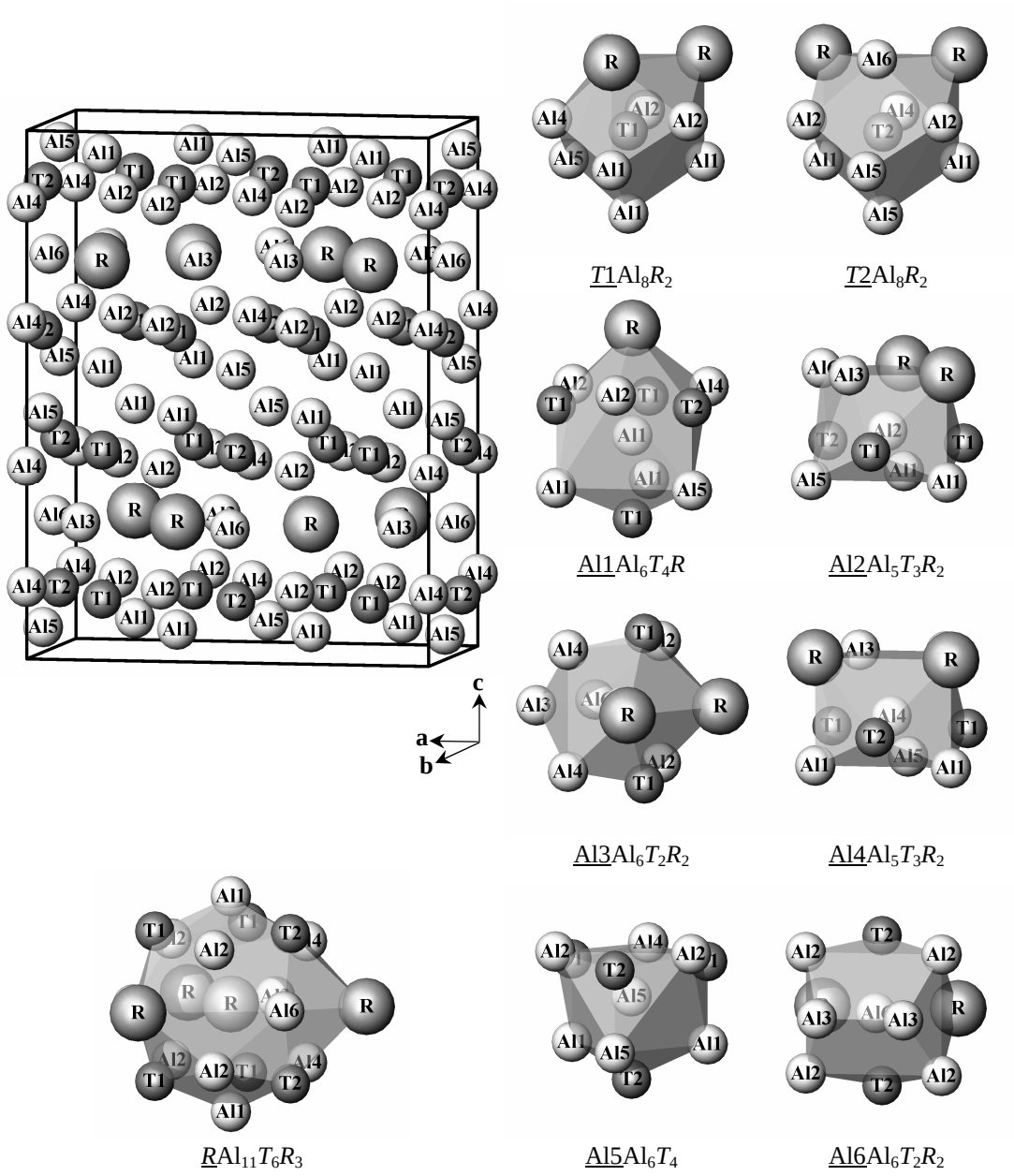

Fig. 4 Content of the unit cell and coordination polyhedra of the atoms for the hypothetical structure $R_2T_6Al_{15}$.

$R_{0.67}Ni_2Al_6$ (space group $P\bar{6}m2$) with statistical arrangement of R atoms and Al_3 triangles is $R_{0.67}$Al-$NiAl_2$-Al-$NiAl_2$. Rhombohedral $DyNi_3Al_9$ and $ErNi_3Al_9$ ($R32$) are partly and fully ordered derivatives of $R_{0.67}Ni_2Al_6$, respectively. The stacking sequence mentioned above repeats three times in the triple-hexagonal cell.

Conclusions

Several members of the homologous series of structures $R_{0.67}T_nM_{2n+1}$ (n = 1, 1.5, and 2) are found among ternary aluminides with a rare earth and a transition metal. The series is based on an intergrowth of two kinds of slab: slightly puckered layers of composition TM_2 and monoatomic layers of composition $R_{0.67}M$. In "consecutive" $R_{0.67}M$ layers the relative orientation of the M_3 triangles is alternatively "up" and "down". Ordered and disordered structures are known, the positions of R atoms and M_3 triangles being in the latter represented by a statistical mixture.

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