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Crystal structure of the new ternary aluminide $CeRu_{3-x}Al_{10+x}$ ($x = 0.17$)

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Abstract

The ternary intermetallic compound $CeRu_{3-x}Al_{10+x}$ ($x = 0.17$) crystallizes in the orthorhombic system, space group *Imma*, $a = 4.2213(1)$ Å, $b = 12.5014(3)$ Å, $c = 17.6689(4)$ Å, $Z = 4$. It is closely related to $NdCo_3Ga_9$ and can be regarded as a substructure of $U_2Co_6Al_{19}$. Trigonal prismatic and cuboctahedral coordination is typical for Al and Ru atoms, the coordination polyhedron of the Ce atom is a pentagonal prism with five additional atoms. The structure can be described as a 3D network of aluminium and ruthenium atoms, forming distorted pentagonal channels along [1 0 0], where the cerium atoms are located.
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Keywords: Cerium ruthenium aluminide; Crystal structure; $CeRu_{3-x}Al_{10+x}$

1. Introduction

Systematic studies of X-ray powder diffraction patterns of the alloys from the Ce–Ru–Al ternary phase diagram allowed us to establish the existence of four ternary intermetallic compounds with high aluminium content. Recently, crystal structures of three of them were determined from single-crystal X-ray diffraction data [1–3]. The compound $Ce_3Ru_4Al_{12}$ [1] adopts the $Nd_3Ru_4Al_{12}$ structure type [4], $CeRu_2Al_{10}$ [2] crystallizes with the $YbFe_2Al_{10}$ structure type [5], and $Ce_2Ru_3Al_{15}$ [3] is of a new type of intermetallic compound. This paper presents the results of the structure determination of the new ternary aluminide $CeRu_{3-x}Al_{10+x}$ ($x = 0.17$).

2. Experimental procedure

A single crystal for the structure determination was extracted from the surface of the alloy with the nominal $Ce_{10}Ru_{10.5}Al_{79.5}$ composition. The sample with a total mass of 1 g was prepared by arc melting of the high purity elements (Ce 99.85 wt.%, Ru 99.96 wt.%, Al 99.99 wt.%) under an argon atmosphere. Weight loss was less than 1%. The sample was annealed at 600 °C for 1 month in a quartz tube under vacuum then quenched in cold water.

Intensity diffraction data were collected on a Nonius Kappa CCD four-circle diffractometer (Mo Kα radiation, ω-scan). The crystallographic and experimental data are given in Table 1.

The systematic extinction rules allow two space groups *Imma* and *Ima*2, of which the group *Imma* was found to be correct during the structure refinement. The positions of the atoms were determined by direct methods using SHELXS-97 [6]. The structure was refined by SHELXL-97 [6] with anisotropic displacement parameters for all atoms to the residual values of $R = 0.029$, $R_w = 0.068$. The atomic parameters were standardized with the program STRUCTURE TIDY [7]. Positional and thermal parameters are listed in Table 2; selected interatomic distances are given in Table 3.

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Table 1
Data collection and structure refinement parameters for $CeRu_{3-x}Al_{10+x}$ ($x = 0.17$) structure

Space group	*Imma*
Lattice parameters	$a = 4.2213(1)$ Å, $b = 12.5014(3)$ Å, $c = 17.6689(4)$ Å
Cell volume	923.43(3) (Å^3)
Formula per unit cell	4
Calculated density	5.080 (g/cm^3)
Scan range	$3.26^\circ \le \theta \le 40.41^\circ$
Linear absorption coefficient	10.429 (mm^{-1})
Range in $h\,k\,l$	$-7 \le h \le 6$, $-22 \le k \le 22$, $-29 \le l \le 32$
Symmetry-independent reflections	1682
Reflections with $F_o > 4\sigma F_o$	1523
Number of refined parameters	55
Goodness of fit	1.086
R	0.029
R_w	0.068

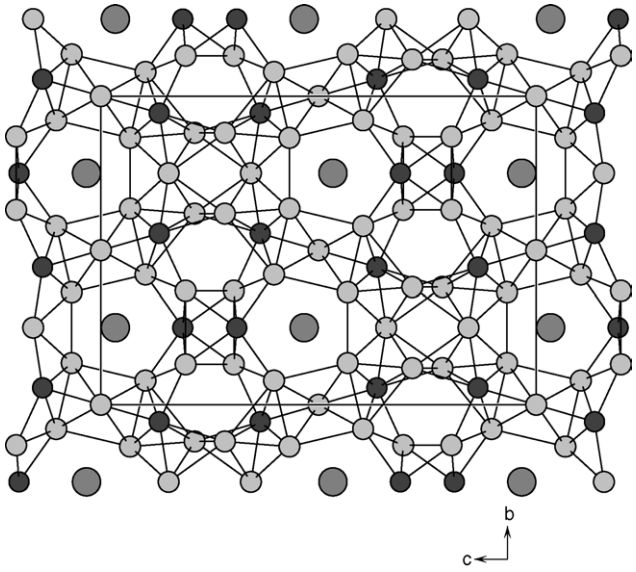

Fig. 1. Projection of the structure $CeRu_{3-x}Al_{10+x}$ on to the 0–y–z plane with Ce atoms shown as big light grey circles, Ru atoms as dark grey circles and Al atoms as middle grey circles. Atom Al1 has been omitted for clarity. The unit cell is outlined.

3. Discussion

All atomic sites are occupied by only one atom sort except M, which is statistically occupied by ruthenium and aluminium M = 0.83Ru + 0.17Al.

The interatomic distance Al1–Al3 is equal to 0.891(4) Å. This indicates that these atoms cannot concurrently reside in the unit cell. Indeed, the refinement of the occupancies of Al1 and Al3 sites gives the values close to 0.5, suggesting a possible superstructure. However, careful examination of some selected reciprocal planes from the collected data did not evidence superstructure peaks towards the initial orthorhombic cell. Consequently, the structure $CeRu_{3-x}Al_{10+x}$ (I), along with the structure of $NdCo_3Ga_9$ (II) [8], can be regarded as substructures of the $U_2Co_6Al_{19}$ structure (space group $C2/m$, $a = 17.4617(3)$ Å, $b = 12.0474(2)$ Å, $c = 8.2003(1)$ Å, $\beta = 103.915^\circ$) [9].

Trigonal-prismatic and cuboctahedral type of coordination are typical for the lower size atoms, aluminium and ruthenium atoms. The trigonal prisms of the Al1, Ru1 and Al3 atoms are capped by four additional atoms. The coordination polyhedra of Al2, Al4, Al5, Al7, and M are deformed cuboctahedra. The coordination environment of the Al6 atom is quite irregular as six disordered Al3(Al1) atoms are among its nearest neighbors. The Ce atom is at the center of a pentagonal prism with five additional atoms capping all side faces of the prism.

The $CeRu_{3-x}Al_{10+x}$ structure can be described as a three-dimensional network of aluminium and ruthenium atoms, forming distorted pentagonal channels along [1 0 0] where the cerium atoms are located (Fig. 1).

The structure $CeRu_{3-x}Al_{10+x}$ is closely related to the $NdCo_3Ga_9$ structure. The difference between the structures I and II lies, firstly, in the additional atom position in I. In II, Co1 atom is located in 8h Wyckoff position with occupancy 0.5, whereas in I, two Al atoms are in 8h sites with occupancy of 0.5. Secondly, the crystallographic positions, occupied in II by Co and Ga atoms do not fully coincide with the positions of Ru and Al atoms in I, respectively.

Table 2
Atomic coordinates and anisotropic displacement parameters (Å^2)

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{23}[a]
Al1[b]	8h	0	0.0476(2)	0.28368(14)	0.0065(9)	0.0226(13)	0.0060(8)	0.0035(8)
Ru1	8h	0	0.05497(2)	0.13394(2)	0.00485(10)	0.00519(10)	0.00505(10)	0.00022(6)
Al2	8h	0	0.07858(12)	0.60241(9)	0.0075(5)	0.0139(5)	0.0266(7)	−0.0082(5)
Al3[b]	8h	0	0.1189(3)	0.28470(14)	0.0052(8)	0.0248(14)	0.0078(9)	−0.0016(9)
Al4	8h	0	0.13548(10)	0.43298(7)	0.0062(4)	0.0083(4)	0.0133(5)	−0.0027(4)
Al5	8h	0	0.63102(11)	0.19465(7)	0.0106(5)	0.0136(5)	0.0120(5)	−0.0057(4)
Al6	4e	0	0.25	0.15552(11)	0.0146(7)	0.0052(6)	0.0158(7)	0
M	4e	0	0.25	0.68809(3)	0.00930(19)	0.00502(17)	0.00837(18)	0
Ce	4e	0	0.25	0.96687(2)	0.00837(11)	0.00777(11)	0.00833(11)	0
Al7	4a	0	0	0	0.0142(7)	0.0140(7)	0.0075(6)	−0.0025(5)

[a] $U_{12} = U_{13} = 0$ for all atoms.
[b] Site occupation of atoms Al1 and Al3 is equal to 0.5.

Table 3
Selected interatomic distances in $CeRu_{3-x}Al_{10+x}$ (Å)

Atom	To atom	*d*
Al1	2 Al1	2.423(2)
	2 Al3	2.590(2)
	Al2	2.557(3)
	2 Ru1	2.5655(14)
	Ru1	2.647(3)
	Al5	2.732(3)
	Al4	2.857(3)
	2 Al5	3.097(3)
Ru1	Al7	2.4643(2)
	Al6	2.4678(4)
	Al5	2.5607(13)
	2 Al1	2.5655(14)
	2 Al3	2.6759(17)
	2 Al4	2.6203(7)
	Al1	2.647(3)
	Al3	2.781(3)
	2 Al2	2.7480(10)
Al2	Al1	2.557(3)
	Al3	3.174(3)
	M	2.6238(14)
	2 Al5	2.7461(13)
	Al4	2.7481(19)
	2 Ru1	2.7481(10)
	2 Al7	2.9486(10)
	Al4	3.077(2)
	2 Ce	3.2475(13)
Al3	2 Al3	2.441(3)
	2 Al1	2.590(2)
	Al4	2.628(3)
	2 Ru1	2.6759(17)
	Ru1	2.781(3)
	Al6	2.810(3)
	2 Al6	2.873(2)
	Al2	3.174(3)
Al4	2 Ru1	2.6203(7)
	Al3	2.628(3)
	Al1	2.857(3)
	Al2	2.7481(19)
	Al4	2.863(3)
	2 Al7	2.9540(9)
	2 Al6	2.9915(14)
	Al2	3.077(2)
	2 Ce	3.1041(9)
Al5	M	2.5504(13)
	Ru1	2.5607(13)
	2 M	2.5847(8)
	Al1	2.732(3)
	2 Al2	2.7461(13)
	2 Al5	2.8775(18)
	Al5	2.975(3)
	2 Al1	3.097(3)
	Ce	3.2183(14)
Al6	2 Ru1	2.4678(4)
	2 Al3	2.810(3)
	2 Al1	3.395(3)
	4 Al3	2.873(2)
	4 Al1	3.465(3)
	4 Al4	2.9915(14)
	Ce	3.333(2)
M	2 Al5	2.5504(13)
	4 Al5	2.5847(8)
	2 Al2	2.6238(14)
	2M	3.0400(7)
	2 Ce	3.4571(4)
Ce	4 Al4	3.1041(9)
	2 Al7	3.1797
	2 Al5	3.2183(14)
	4 Al2	3.2475(13)
	Al6	3.333(2)
	2 M	3.4571(4)
Al7	2 Ru1	2.4643(2)
	4 Al2	2.9486(10)
	4 Al4	2.9540(9)
	Ce	3.1797

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