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Mo-PO9

Novel ternary gallides of the structural family Ce_{2+n}Rh_{3+3n}Ga_{1+2n}(n=0÷6)*

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The direct alloying of cerium, rhodium, and gallium results in the formation of intermetallic compounds with sequence of related structures, forming a new homologous series. Structures of 9 ternary intermetallic compounds of Ce-Rh-Ga system containing 50 at.% of rhodium were determined from single-crystal X-ray diffractometer data. The compounds are built up of columns of alternating combination of the fragments of Ce₂Rh₃Ga with Mg₂Cu₃Si structure (MgZn₂-type) or Mg₂Ni₃Si (MgCu₂-type) and fragments of CeRh₃Ga₂ with CeCo₃B₂ structure (CaCu₅-type), forming the homologous series R_{2+n}T_{3+3n}M_{1+2n} (*n*=0÷6). They can be grouped in two different structural series: trigonal (*R*-3*m*) and hexagonal (*P*6₃/*mmc*) group, depending on Laves-type fragment.

n=0	Ce ₂ Rh ₃ Ga	<i>R</i> -3 <i>m</i>	Z=3	<i>a</i> =5.614(2)	<i>c</i> =11.932(5)
n=1	CeRh ₂ Ga	P6 ₃ /mmc	6	a=5.556(3)	<i>c</i> =15.680(8)
n=2	Ce ₄ Rh ₉ Ga ₅	<i>R</i> -3 <i>m</i>	3	a=5.554(3)	<i>c</i> =34.98 (2)
n=3	trig-Ce ₅ Rh ₁₂ Ga ₇	<i>R</i> -3 <i>m</i>	3	<i>a</i> =5.563(4)	<i>c</i> =46.36(6)
	hex-Ce ₅ Rh ₁₂ Ga ₇	P6 ₃ /mmc	2	<i>a</i> =5.597(3)	<i>c</i> =31.40(3)
n=4	trig -Ce ₂ Rh ₅ Ga ₃	<i>R</i> -3 <i>m</i>	3	<i>a</i> =5.5743(8)	<i>c</i> =57.82 (2)
	hex-Ce ₂ Rh ₅ Ga ₃	P6 ₃ /mmc	6	<i>a</i> = 5.5923(12)	<i>c</i> = 38.116(10)
n=5	Ce7Rh18Ga11	<i>R</i> -3 <i>m</i>	3	<i>a</i> =5.583(2)	<i>c</i> =69.35(3)
n=6	Ce ₈ Rh ₂₃ Ga ₁₁	<i>R</i> -3 <i>m</i>	3	<i>a</i> =5.571 (3)	<i>c</i> =80.53 (3)

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Mo-PO10

Novel ternary aluminide Ce₄Ru₃Al₂*

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The crystal structure of a novel ternary intermetallic aluminide Ce₄Ru₃Al₂ was determined from the synchrotron X-ray powder diffraction data collected on an almost single-phase alloy. The compound crystallizes with an orthorhombic structure of new type: space group *Pnma*, lattice parameters a = 22.0592(5), b = 4.62213(6), c = 4.67.54309(8) Å, Z = 4. It can be presented as packing of coupled trigonal prisms with Ru-atoms located inside the prims and quadrilaterals Ru₂Al₂ residing in between them. The new structure is closely related to those of the equiatomic germanides YbAuGe and CaCuGe [1-2], which have similar atomic order with a total of nine crystallographic sites of the same multiplicity. However, while in the germanides, each type of atoms occupies three sites, in Ce₄Ru₃Al₂, Ce atoms are distributed over four sites, Ru atoms occupy three sites, and Al atoms are located at two sites. A remarkable feature of Ce₄Ru₃Al₂ is extremely small values of some Ce-Ru distances, ranging from 2.300(1) to 2.572(1) Å. Only one of the four inequivalent Ce atom exhibits a regular distance from its nearest neighbors, exceeding 3.235(1) Å. In concert with the structural characteristics, Ce₄Ru₃Al₂ was established by means of low-temperature magnetic and electrical transport measurements to exhibit a coexistence of valence fluctuations and local moment magnetism, attributable to the Ce atom sublattices with anomalously short and normal Ce-Ru interatomic distances, respectively. Due to the $\frac{1}{4}$ fraction of Ce³⁺ ions with fairly stable $4t^{4}$ electronic configuration, Ce₄Ru₃Al₂ orders antiferromagnetically at $T_{\rm N} = 2$ K and shows Kondo behavior in its electrical resistivity. In this respect, the novel aluminide resembles the gallide $Ce_9Ru_4Ga_5$ that also bears in its crystallographic unit cell Ce ions with diverse valence states [3].

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^[1] F. Merlo et al., J. Alloys Compd. 264 (1998) 82

^[2] W. Dörrscheidt et al., Z. Naturforschung 32 (1977) 985

^[3] D. Kaczorowski et al., J. Alloys Compd. 557 (2013) 23

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