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New ternary silicide of cerium and palladium Ce_3Pd_5Si

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Abstract

The crystal structure of the new compound Ce_3Pd_5Si was investigated by X-ray single crystal diffraction method. The compound crystallizes in a new structure type, space group *Imma* $Z=4$, $a=1.3027(4)$ nm, $b=0.7377(4)$ nm, $c=0.7580(4)$ nm. © 2001 Elsevier Science B.V. All rights reserved.

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1. Introduction

The unusual physical properties of the known R–T–X intermetallic compounds have become the reason for intensive study of the ternary phase diagrams R–T–X (R, rare earth; T, transition metal; X, element from the III or IV main group), with the purpose of definition of crystal structure and low-temperature properties of new ternary phases.

The ternary system Ce–Pd–Si had not been studied through the whole concentration range before our work. When investigating the Ce–Pd–Si system we established the existence of a few ternary intermetallics, and here data is presented for one of them — Ce_3Pd_5Si.

2. Experimental details

A single crystal used for the crystal structure determination of the new phase was extracted from an ingot of the $Ce_{33}Pd_{57}Si_{10}$ composition. This alloy of 1 g was prepared by melting in an arc furnace in an argon atmosphere. The purity of the starting metals was better than 99%. The homogenization annealing was done at 870 K during 720 h. A sample of alloy was examined by DTA, X-ray single crystal and powder diffraction methods. DTA was performed in an Al_2O_3 crucible with W/W(20% Re) thermocouples and speed of heating 80 deg./min. A single crystal was examined photographically and then using an Enraf-Nonius CAD-4 automatic diffractometer (Mo K_α-radiation, flat graphite monochromator, ω–2θ scanning). The calculation was performed using 334 independent reflections with $I_0 = 4\sigma(I_0)$.

The X-ray powder diffraction experiment was done with DRON-3,0 equipment (Cu K_α radiation, step 0.1°).

3. Results and discussion

DTA indicates the melting temperature of the $Ce_{33}Pd_{57}Si_{10}$ alloy to be 985 ± 5°C.

Inasmuch as the annealing of the ingot does not result in the formation of single crystals suitable for X-ray analysis, we undertook attempts to get these by slow cooling from the melting temperature. Single crystal was found just in that part of the alloy which did not contact with the wall of the crucible.

X-ray single crystal experiment conditions and results are summarized in Tables 1–4.

Coordination polyhedra of the Ce atoms are distorted cubes with one additional atom $Ce1[Pd_8Si_1]$ and polyhedra with 10 apexes $Ce2[Pd_{10}]$. Coordination polyhedra of the Pd atoms have 6 and 8 apexes: $Pd1[Ce_4Si_2]$ — quadrangles with two additional atoms, and $Pd2[Ce_6SiPd]$ — distorted trigonal prisms with two additional atoms. Si1 atoms have polyhedra with 6 apexes: $Si[Pd_6]$ — trigonal prisms, which are typical for Si. The unit cell of Ce_3Pd_5Si with coordination polyhedra of the Si1 atoms is given in Fig. 1.

The powder X-ray diffraction method shows that this

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Table 1
Experimental details obtained from single crystal X-ray experiment

Space group	*Imma*
a, (nm)	1.3027(4)
b, (nm)	0.7377(4)
c, (nm)	0.7580(4)
Cell volume (nm^3)	0.728(1)
Z	4
$D_{calc.}$ ($g\ cm^{-1}$)	8.94(1)
Radiation	Monochromatized Mo K_α, $\lambda = 0.071069$ nm
Diffractometer	DARTCH
Absorption coefficient (μ, cm^{-1})	303.28
Scan technique	$\omega - 2\theta$
Two-theta max. (deg.)	69.32
Data collection *h*, *k*, *l*	$0 \leq h \leq 20$, $0 \leq k \leq 10$, $0 \leq l \leq 11$
Number of measured reflections	555
Reflection used in refinement	334
Number of refined parameters	29
Restrictions	$\lvert F_0 \rvert \geq 4\sigma \lvert F_0 \rvert$
R	0.0223

Table 2
Atomic coordinates and equivalent displacement parameters of Ce_3Pd_5Si

Site	Occupancy	*X*	*Y*	*Z*	$B_{eq.}$
4*e*	4 Ce1	0	1/4	0.3856(2)	0.84(3)
8*i*	8 Ce2	0.19997(7)	1/4	0.0230(1)	0.69(2)
4*a*	4 Pd1	0	0	0	1.63(5)
16*j*	16 Pd2	0.14327(7)	0.0502(1)	0.6868(1)	0.92(2)
4*e*	4 Si1	0	1/4	0.7886(9)	1.0(2)

Table 3
Anisotropic displacement parameters B_{ij} for Ce_3Pd_5Si

Name	*B*(1,1)	*B*(2,2)	*B*(3,3)	*B*(1,2)	*B*(1,3)	*B*(2,3)
Ce1	0.61(5)	0.90(5)	1.01(6)	0	0	0
Ce2	0.72(3)	0.63(3)	0.71(3)	0	−0.04(3)	0
Pd1	0.85(7)	2.60(8)	1.45(9)	0	0	1.12(7)
Pd2	1.08(3)	0.84(3)	0.83(3)	−0.13(3)	0.05(3)	−0.16(3)
Si1	0.5(2)	1.3(2)	1.1(3)	0	0	0

Table 4
Interatomic distances in the structure of Ce_3Pd_5Si

Atom 1	Atom 2	Distance (nm)	Atom 1	Atom 2	Distance (nm)
Ce1	4 Pd2	0.2947(4)	Pd1	2 Ce1	0.3456(4)
Ce1	1 Si1	0.3055(8)	Pd2	1 Si1	0.2500(5)
Ce1	4 Pd2	0.3297(4)	Pd2	1 Pd2	0.2926(4)
Ce1	2 Pd1	0.3456(4)	Pd2	1 Pd2	0.2942(4)
Ce1	2 Ce2	0.3787(4)	Pd2	1 Ce1	0.2947(4)
Ce2	2 Pd2	0.2978(4)	Pd2	1 Pd2	0.2948(4)
Ce2	2 Pd2	0.3035(4)	Pd2	1 Ce2	0.2978(4)
Ce2	1 Si1	0.3153(6)	Pd2	1 Ce2	0.3035(4)
Ce2	2 Pd1	0.3196(4)	Pd2	1 Pd1	0.3043(4)
Ce2	2 Pd2	0.3208(4)	Pd2	1 Ce2	0.3208(4)
Ce2	2 Pd2	0.3258(4)	Pd2	1 Ce2	0.3258(4)
Ce2	1 Ce2	0.3680(4)	Pd2	1 Ce1	0.3297(4)
Ce2	2 Ce2	0.3705(4)	Si1	2 Pd1	0.2443(6)
Ce2	1 Ce1	0.3787(4)	Si1	4 Pd2	0.2500(5)
Pd1	2 Si1	0.2443(6)	Si1	1 Ce1	0.3055(8)
Pd1	4 Pd2	0.3043(4)	Si1	2 Ce2	0.3153(6)
Pd1	4 Ce2	0.3196(4)			

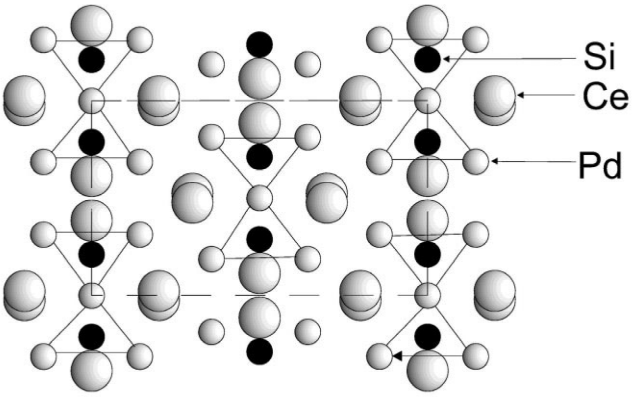

Fig. 1. Projection of a unit cell of the Ce_3Pd_5Si structure onto *XZ*-plane and coordination polyhedra of the Si1 atoms.

compound is not the single phase in the ingot after arc melting and annealing. Some amount of $CePd_3$ is presented. Therefore we assume that Ce_3Pd_5Si does not form from liquid phase directly.

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