

Crystal structure of the new ternary silicide CePt₃Si

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Abstract

The crystal structure of the new ternary silicide CePt₃Si [space group *P4mm*, *a* = 4.072(1) Å, *c* = 5.442(2) Å, *Z* = 1, *V* = 90.25(5) Å³, *R* = 0.0437 for 153 structure factors] was determined from single-crystal X-ray diffraction. The compound belongs to the CePt₃B structure type of intermetallic compounds.

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1. Introduction

In the system Ce–Pt–Si four ternary compounds with different structure types are found: CePtSi₂ (CeNiSi₂ structure type, space group *Cmcm*) [1], CePt₂Si₂ (CaBe₂Ge₂ structure type, *P4/nmm*) [2], CePtSi (LaPtSi structure type, *I4₁md*) [3], and Ce₃Pt₂₃Si₁₁ (Ce₃Pt₂₃Si₁₁ structure type, *Fm-3m*) [4]. During our investigation of this phase diagram the existence of a new silicide has been established.

2. Experimental details

A ternary sample of the composition Ce:Pt:Si = 20:60:20 was synthesized by arc-melting of the constituent high purity elements under an argon atmosphere on a water-cooled copper hearth. The weight loss during arc-melting was less than 1%. The sample was wrapped in nickel foil, sealed in a double quartz ampoule, and annealed at 870 K for 30 days and then quenched in cold water to room temperature.

The sample was then examined by differential thermal analysis on a VDTA-8M2 device in an Al₂O₃ crucible with a W/(W80%–Re20%) thermocouple with heating and cooling rates of 2.5 °C/min and characterized by X-ray powder

diffraction using a Guinier–Huber diffractometer with monochromatic Cu Kα₁ radiation.

A single crystal with the dimensions 0.06 mm × 0.06 mm × 0.06 mm suitable for the X-ray measurements was isolated from the surface of the alloy. X-ray data were collected on a Nonius Kappa CCD diffractometer with monochromatized Mo Kα radiation. The structure was solved in space group *P4mm* and refined by a full-matrix least-squares program [5]. No absorption correction was applied. Further details are listed in Table 1.

3. Results and discussion

Differential thermal analysis indicated only one thermal effect at *T* = 1390 ± 10 °C, which corresponds to the final melting. X-ray powder diffraction data clearly showed that the sample contained the compound CePt₃Si as a single phase. The ternary compound CePt₃Si crystallizes with CePt₃B structure type (space group *P4mm*, *a* = 4.00433 Å, *c* = 5.07547 Å) [6]. Refined atomic coordinates, anisotropic displacement parameters, and interatomic distances for the structure are presented in Tables 2–4.

The crystal structure of CePt₃Si compound and the coordination polyhedra of the atoms are shown in Figs. 1 and 2, respectively. In the CePt₃Si structure, each cerium atom has 16 nearest neighbors—12 platinum and four silicon atoms [Pt₁₂Si₄] (Fig. 2a). Pt1 is in the center of distorted trigonal

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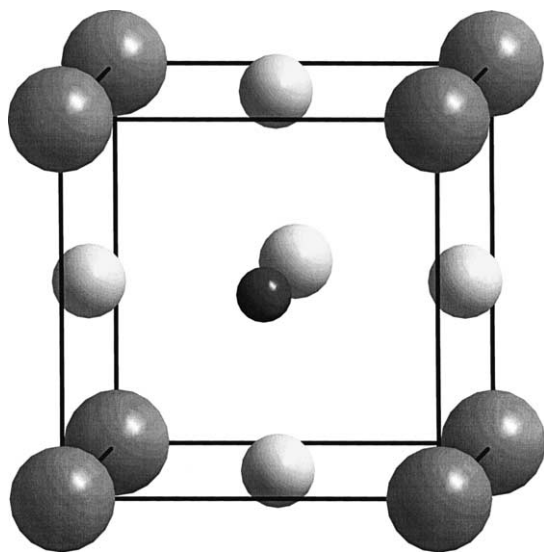


Fig. 1. View of the structure of CePt_3Si . Large size circles indicate Ce atoms, Pt and Si atoms are marked by middle and small size circles, respectively.

Table 1

Crystallographic data and experimental conditions for the structure refinement of CePt_3Si

Space group	$P4mm$
a (Å)	4.072(1)
c (Å)	5.442(2)
Cell volume (Å ³)	90.25(5)
Z	1
D_{calc} (g cm ⁻³)	13.864
Absorption coefficient (μ , mm ⁻¹)	128
Extinction coefficient	0.006(3)
Scan range (°)	$3.74 \leq \theta \leq 36.36$
Data collection (h, k, l)	0–6, 0–6, 0–9
Number of measured reflections	1426
Independent reflections	164
Reflections used in refinement ($F_o > 2\sigma(F_o)$)	153
Number of refined parameters	14
$R(F)$	0.044

prism with three additional atoms (two Pt and one Si atom), which cap the tetra-angular faces of the prism [$\text{Ce}_4\text{Pt}_4\text{Si}$] (Fig. 2b). The Pt2 atom is coordinated by a distorted tetragonal prism of six platinum and two silicon atoms [Pt_6Si_2]

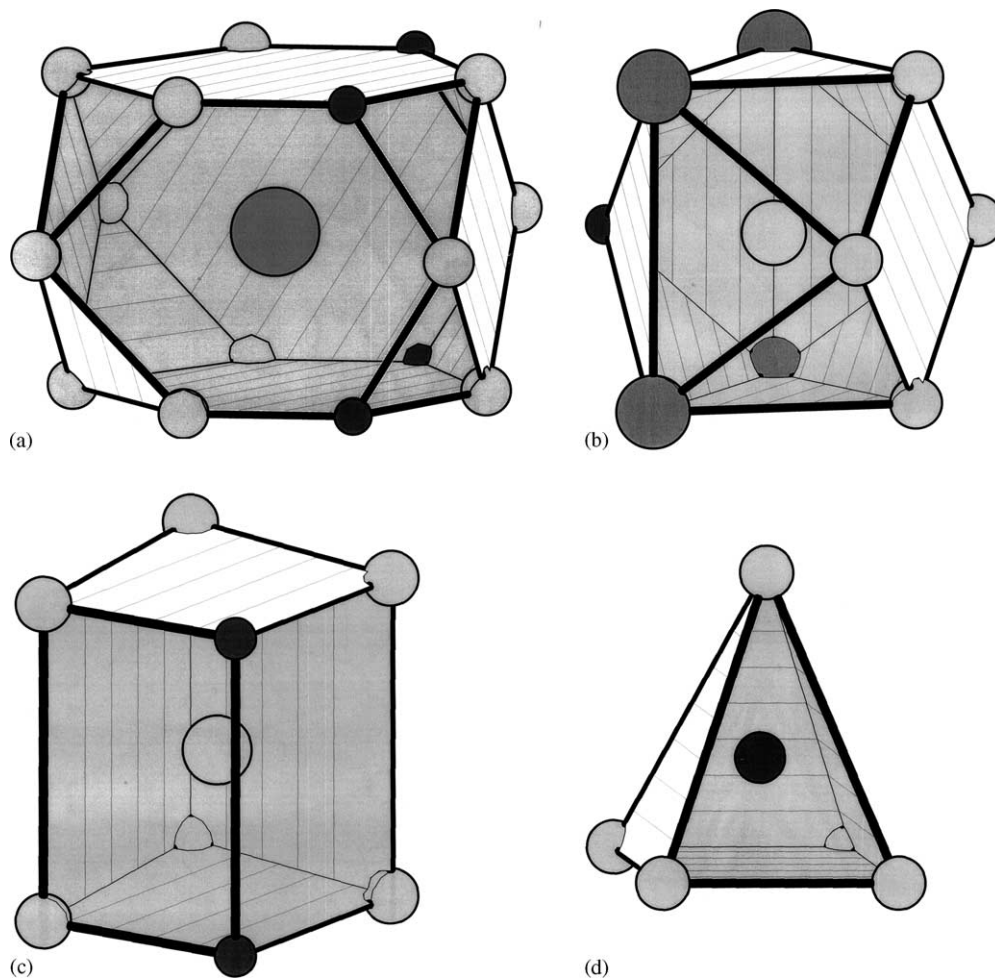


Fig. 2. Coordination polyhedra for Ce (a), Pt1 (b), Pt2 (c), and Si (d) atoms.

Table 2
Atomic coordinates and equivalent isotropic displacement parameters ($\text{\AA}^2$) for CePt_3Si

Atom	x	y	z	U_{eq}
Ce	0	0	0	0.0048(5)
Pt1	1/2	1/2	0.1468(6)	0.0041(4)
Pt2	1/2	0	0.4964(6)	0.0034(4)
Si	1/2	1/2	0.735(3)	0.001(2)

Table 3
Anisotropic displacement parameters ($\text{\AA}^2$) for CePt_3Si

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ce	0.0040(6)	0.0040(6)	0.0064(13)	0	0	0
Pt1	0.0045(5)	0.0045(5)	0.0032(7)	0	0	0
Pt2	0.0047(5)	0.0009(5)	0.0044(6)	0	0	0
Si	0.002(3)	0.002(3)	0.000(4)	0	0	0

Table 4
Interatomic distances ($\text{\AA}$) in the structure of CePt_3Si

Atom1	Atom2	Distance	Atom1	Atom2	Distance
Ce	4 Pt1	2.988(1)	Pt2	2 Si	2.416(9)
	4 Si	3.219(8)		2 Pt1	2.787(2)
	4 Pt2	3.383(3)		4 Pt2	2.880(1)
	4 Pt2	3.414(3)		2 Ce	3.383(3)
Pt1	Si	2.24(2)	Si	2 Ce	3.414(3)
	4 Pt2	2.787(2)		Pt1	2.24(2)
	4 Ce	2.988(1)		4 Pt2	2.416(9)

Table 5
Unit-cell dimensions for REPt_3Si phases with CePt_3B structure type

REPt_3Si	a ($\text{\AA}$)	c ($\text{\AA}$)	V ($\text{\AA}^3$)
LaPt_3Si	4.115(1)	5.438(2)	92.06(4)
NdPt_3Si	4.0485(9)	5.436(2)	89.10(2)
SmPt_3Si	4.034(3)	5.411(7)	88.06(9)

(Fig. 2c). The coordination polyhedron of Si atom is a tetragonal pyramid of five platinum atoms (Fig. 2d).

The CePt_3Si compound is the first example of a silicide of $\text{RE-T}_3\text{-Si}$ composition (RE = rare earth, T = transition metal). Investigated earlier carbides and borides RET_3X ($\text{X} = \text{C}, \text{B}$) had perovskite type of structure [7] except the recently described compound CePt_3B [6].

The powder diagrams of the NdPt_3Si , LaPt_3Si , and SmPt_3Si compounds (Günier–Huber diffractometer) could be indexed unambiguously assuming the compounds to be of the CePt_3B structure type [6]. The lattice parameters, given in Table 5, were obtained by least-squares refinement of the powder patterns with the aid of the STOE WinXPOW program [8].

Acknowledgements

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References

- [1] W.H. Lee, K.S. Kwan, P. Klavins, R.N. Shelton, Phys. Rev. 42B (1990) 6542.
- [2] A. Dommann, F. Hulliger, H.R. Ott, J. Less-Common Metals 110 (1985) 331.
- [3] K. Klepp, E. Parthé, Acta Crystallogr. B38 (1982) 1105.
- [4] A.I. Tursina, A.V. Gribanov, Y.D. Seropegin, K.V. Kuyukov, O.I. Bodak, J. Alloys Compd. 347 (2002) 121.
- [5] G.M. Sheldrick, SHELXS97 and SHELXL97, University of Göttingen, Göttingen, 1997.
- [6] O.L. Sologub, J.R. Hester, P.S. Salamaakha, E. Leroy, C. Godart, J. Alloys Compd. 337 (2002) 10.
- [7] P. Villars, Pearson's Handbook, Desk Edition, Crystallographic Data for Intermetallic Phases, ASM International, 1997.
- [8] Stoe & Cie, STOE WinXPOW (Version 1.06), Stoe & Cie GmbH, Darmstadt, Germany, 1999.