Short Communications

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The crystal structure of β-$PuSi_2$.

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Plutonium silicides have been prepared by heating 150 mg. charges of plutonium trifluoride, 99·8% pure, mixed with the appropriate weight of silicon of 99·99% purity, in BeO crucibles at 5×10^{-5} mm. Hg. At 1300° C. the reaction was complete after 15 min. The resulting SiF_4 had distilled from the reaction zone, leaving a fluoride-free Pu–Si product. The plutonium silicides prepared by this technique were hard and brittle, with silvery metallic lustre.

Table 1. *Powder diffraction data for* β-$PuSi_2$

hk.l	$(\sin^2\theta)_c$	$(\sin^2\theta)_o$	I_o	I_c†
00.1	0·0357	0·0364	*w*	25·9
10.0	0·0525	0·0533	*m*	63·8
10.1	0·0882	0·0890	*s*	108·2
00.2	0·1427	0·1438	*w*	11·1
11.0	0·1576	0·1585	*m*	28·5
11.1	0·1932	0·1944	*m*−	15·7
10.2	0·1952	0·1965	*m*−	21·0
20.0	0·2101	0·2117	*w*	9·3
20.1	0·2458	0·2469	*m*	23·1
11.2	0·3002	0·3014	*m*	20·4
00.3	0·3210	—	Abs.	1·2
20.2	0·3528	0·3542	*m*−	8·0
21.0	0·3677	0·3677	*w*+	7·4
10.3	0·3735	0·3744	*w*+	11·9
21.1	0·4034	0·4042	*m*	20·7
30.0	0·4727	0·4740	*w*	5·0
11.3	0·4786	0·4797	*w*	4·0
30.1	0·5084	0·5111	*m*	3·7
21.2	0·5104			9·7
20.3	0·5311	0·5320	*w*+	7·4
00.4	0·5706	0·5720	*vw*	1·5
30.2	0·6144	0·6158*	*w*+	8·1
10.4	0·6232	0·6247	*vw*	4·0
22.0	0·6303	0·6310	*vw*	4·1
22.1	0·6660	0·6677	*w*−	3·3
31.0	0·6829	0·6836	*vw*	4·4
21.3	0·6875	0·6889*	*m*	13·6
31.1	0·7185	0·7188	*m*−	14·1
11.4	0·7282	0·7297	*w*+	8·5
22.2	0·7717	0·7720*	*w*+	9·1
20.4	0·7808	0·7822	*w*	4·9
30.3	0·7924	0·7929*	*w*+	4·0
31.2	0·8241	0·8248*	*m*	11·1
40.0	0·8404	0·8407	*w*−	2·8
40.1	0·8746	0·8743*	*m*	10·2
00.5	0·8916	—	Abs.	0·9
21.4	0·9368	0·9366*	*m*+	19·1
10.5	0·9426	0·9426*	*m*	15·3
22.3	0·9497	0·9497*	*m*	8·5

* Cu $K\alpha_1$ reflection.

† $I \propto |F|^2 p \dfrac{1+\cos^2 2\theta}{\sin^2\theta\cos\theta}$.

Since the observed and calculated intensities are in reasonable agreement it may be concluded that β-$PuSi_2$ has the AlB_2 structure. Each plutonium atom is surrounded by twelve silicon atoms, at a distance of 3·03 Å. Each silicon atom is surrounded by six plutonium atoms and three silicon atoms with Si–Si = 2·24 Å. As pointed out by Zachariasen for β-USi_2, in this structural arrangement the silicon atoms form 'graphite layers' normal to the sixfold axis.

An X-ray powder pattern from a product containing 80 wt.% Pu, as determined by α-counting analysis, showed diffraction lines similar to those published by Zachariasen (1949) for body-centred tetragonal $PuSi_2$. A sample with a Si:Pu atom ratio of 3:1 showed diffraction lines of both $PuSi_2$ and Si. Heat treatment of the latter product for 1 hr. at 1150° C. failed to produce a change in the structure. Thus, a plutonium silicide isomorphous with the face-centred cubic USi_3 reported by Frost & Maskrey (1953) could not be formed.

Powder diffraction patterns obtained from Pu–Si products of approximate composition Pu_2Si_3, using Ni-filtered Cu radiation, showed a single hexagonal phase with lattice constants

$$a_0 = 3{\cdot}884\pm0{\cdot}003, \quad c_0 = 4{\cdot}082\pm0{\cdot}003 \text{ Å}.$$

The line spacings and intensities were similar to those published for a uranium silicide, nominally of composition U_2Si_3, but described by the formula β-USi_2 as a result of Zachariasen's X-ray analysis (1949). The Pu–Si phase has been labelled β-$PuSi_2$, to conform with the latter terminology.

The calculated density of β-$PuSi_2$, assuming one molecule per unit cell, is 9·18 g.cm.$^{-3}$. Powder diffraction data are reported in Table 1, together with calculated intensities based on the following atom positions in space group $P6/mmm$–D^1_{6h}:

1 Pu in (0, 0, 0),
2 Si in $(\frac{1}{3}, \frac{2}{3}, \frac{1}{2})$, $(\frac{2}{3}, \frac{1}{3}, \frac{1}{2})$.

References

Frost, B. R. T. & Maskrey, J. T. (1953). *J. Inst. Metals*, **8**, 177.

Zachariasen, W. H. (1949). *Acta Cryst.* **2**, 94.