Acta Cryst. (1961). **14**, 1095

The phase C16 type in the thorium-palladium alloy system.

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(*Received* 10 *April* 1961 *and in revised form* 29 *May* 1961)

During researches on thorium–palladium alloys, the formation was observed, in the thorium-rich part of the system, of a phase corresponding to the structural C16 type (Pearson, 1958) or $CuAl_2$ type (Bradley & Jones, 1933).

The thorium used (Ferro, 1958), was of a purity about 99·7% (the impurities were represented by oxygen in the form of ThO_2); the palladium was of a purity not less than 99·9%. The alloys were prepared by heating the metals up to ca. 1800 °C. in argon (although the melting points for the alloys seem lower); then the samples, still in argon atmosphere, were annealed for one day at 900 °C., 7 days at 750 °C. and 15 days at 500 °C. The filings used for the X-ray examination were further annealed at 500 °C. for ca. 2 days.

The alloys were analyzed by dissolving in a mixture of HCl and H_2O_2 followed by treatment with aqua regia, precipitation of Pd with H_2S, re-solution of palladium sulphide and determination of palladium with dimethylglyoxime. In the filtrate, thorium was determined as ThO_2 via the oxalate.

The powder photographs of alloys with compositions around 18% Pd show the existence of a tetragonal phase with constants:

$$a = 7{\cdot}33_0,\ c = 5{\cdot}93_0\ \text{Å},\ c/a = 0{\cdot}80_9\ .$$

(The powder photographs were obtained with the Straumanis arrangement using Fe $K\alpha$ radiation: $K\alpha_1$, $\lambda = 1{\cdot}93597$ Å.)

The structure corresponds to the C16 type with the following atomic positions:

Space group D_{4h}^{18}

4 Pd in (a): $0, 0, \frac{1}{4};\ 0, 0, \frac{3}{4};\ \frac{1}{2}, \frac{1}{2}, \frac{3}{4};\ \frac{1}{2}, \frac{1}{2}, \frac{1}{4}$.

8 Th in (h): $x, \frac{1}{2}+x, 0;\ \bar{x}, \frac{1}{2}-x, 0;\ \frac{1}{2}+x, \bar{x}, 0;$
$\frac{1}{2}-x, x, 0;\ \frac{1}{2}+x, x, \frac{1}{2};\ \frac{1}{2}-x, \bar{x}, \frac{1}{2};$
$x, \frac{1}{2}-x, \frac{1}{2};\ \bar{x}, \frac{1}{2}+x, \frac{1}{2}$.

The micrographic appearance agrees with the hypothesis of the existence of only one phase for a composition near the theoretical one for Th_2Pd (18·69% Pd); also the density (11·5 g.cm.$^{-3}$, for an alloy containing $19{\cdot}4_0$% Pd and $80{\cdot}6_7$% Th) appears in fair agreement with the value calculated on the basis of above structure (11·9 g.cm.$^{-3}$).

The intensities observed on the film were compared with those calculated for different values of x between 0·150 and 0·175. Although, unfortunately, the c/a value results in many coincidences which prevent the exact estimation of the separate contribution of the reflections, the best agreement between observed and calculated intensities seems to be obtained for $x = 0{\cdot}16_0$.

In Table 1 are reported the unit-cell dimensions (Å) and the molar volumes (cm.^{3}), obtained both from crystallographic data (V_M) and by adding the atomic volumes (ΣV_A), for the thorium compounds with this structure. Even considering the fact that many of these phases have probably a small composition range, it can be seen that there are no remarkable volume variations.

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Table 1. *Structural data for* Th_2Me *compounds*

Th_2Me	a	c	c/a	V_M	ΣV_A	References
Th_2Al	7·614	5·857	0·769	51·1	49·7	Braun & van Vucht, 1955; Murray, 1955
Th_2Zn	7·60	5·64	0·74	49·1	48·8	Baenziger *et al.*, 1956
Th_2Cu	7·29	5·75	0·79	46·0	46·8	Murray, 1955; Baenziger *et al.*, 1956
Th_2Ag	7·56	5·84	0·77	50·3	50·0	Murray, 1955
Th_2Pd	7·33	5·93	0·81	48·0	48·6	
Th_2Au	7·42	5·95	0·80	49·3	49·9	Murray, 1955

Acta Cryst. (1961). **14**, 1095

The anomalous temperature behavior of the 200 reflection of fluorite.*

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(*Received* 30 *March* 1961)

On a diffractometer recording of the powder pattern of CaF_2, the area of a peak is expressed in terms of the structure factor squared, the multiplicity, and the Lorentz-polarization factor, by the relation

$$A = K^2(\mathrm{F}/4)^2 m(L\,.\,P)\ .$$

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* Research sponsored by the U.S. Atomic Energy Commission.