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Al–Th intermetallic compounds. II.

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In our previous communication (Braun & van Vucht, 1955) we described the phases Al_3Th, Al_2Th and Al_2Th_3. Now we intend to give some data on three other phases which we have discovered, using the same methods as described previously.

I. AlTh

The powder diagram was indexed with the help of a Weissenberg diagram of a very poor single crystal. Both diagrams helped us to build up a tentative structure as follows:

Space group: $C222_1$ (No. 20);
$a = 11{\cdot}45$, $b = 4{\cdot}42$, $c = 4{\cdot}19$ Å;
$z = 4$;
$d_o = 8{\cdot}10$, $d_c = 8{\cdot}11$ g.cm.$^{-3}$;
Th in $4a$ $(x, 0, 0)$, $(\bar{x}, 0, \frac{1}{2})$, $(\frac{1}{2}+x, \frac{1}{2}, 0)$, $(\frac{1}{2}-x, \frac{1}{2}, \frac{1}{2})$ with $x = 0{\cdot}147$,
Al in $4a$ $(y, 0, 0)$, $(\bar{y}, 0, \frac{1}{2})$, $(\frac{1}{2}+y, \frac{1}{2}, 0)$, $(\frac{1}{2}-y, \frac{1}{2}, \frac{1}{2})$ with $y = 0{\cdot}443$;
$\sum_{54} |I_o - I_c| \div \sum_{54} I_o = 17{\cdot}2\%$.

Again this structure appears to be related to Al_2Th. Plates, built up of Al_2Th-like cells, stretch in the bc planes. The pseudo-hexagonal axis lies in the b direction. Two plates build up the a period, while they are shifted with respect to another over half a period both in the b and c directions. The Al_2Th-like cells are not exactly hexagonal: the angles are 58° 4′ and 63° 52′.

A Th atom has 4Th neighbours at a distance of 3·85 Å, 2Th at 3·96 Å, 2Th at 4·19 Å and 2Th at 4·42 Å. In addition it has 3Al neighbours at 3·22 Å and 1Al at 3·39 Å. The shortest Al–Al distance is 2·46 Å, being still smaller than in Al_2Th.

II. $AlTh_2$

We measured 47 reflexions, only one of which was very strong. We propose the following structure:

Space group: $I4/mcm$ (No. 140);
$a = 7{\cdot}62$, $c = 5{\cdot}86$ Å;
$z = 4$;
$d_o = 9{\cdot}61$, $d_c = 9{\cdot}63$ g.cm.$^{-3}$;
Th in $8h$ $\pm(x, \frac{1}{2}+x, 0)$, $\pm(\frac{1}{2}+x, \bar{x}, 0)$, $\pm(\frac{1}{2}+x, x, \frac{1}{2})$, $\pm(x, \frac{1}{2}-x, \frac{1}{2})$ with $x = 0{\cdot}162$,
Al in $4a$ $\pm(0, 0, \frac{1}{4})$, $\pm(\frac{1}{2}, \frac{1}{2}, \frac{1}{4})$;
Structure type: $C16$ ($CuAl_2$);
$\sum_{47} |I_o - I_c| \div \sum_{47} I_o = 13{\cdot}2\%$.

A Th atom is surrounded by 3Th atoms at a distance of 3·49 Å, 4Th atoms at 3·83 Å and by 4Al atoms at a distance of 3·21 Å. The Al–Al distance is 2·93 Å. Contrary to the other known Al–Th compounds, this has a short Th–Th distance and a long Al–Al distance. Nowotny (1942) described a similar case in the systems Ce–Al and La–Al.

III

The sixth phase in the Al–Th system is stable only in a narrow temperature range at about 1300° C. We have not yet succeeded in isolating it in a pure state. Therefore its composition is not exactly known, though it must lie between that of Al_2Th and AlTh, probably in the neighbourhood of Th_4Al_7. The powder diagram, showing in addition the lines of Al_2Th and AlTh, revealed 23 lines of this phase, which could be indexed on the basis of a tetragonal unit cell with

$$a = 9{\cdot}86,\ c = 7{\cdot}81 \text{ Å}.$$

Data of the first two phases, described here, have been sent to the A. S. T. M. Card Index Committee.

Further investigations of the above mentioned Al–Th compounds must await the production of single crystals, as the parameters cannot be refined further from our powder diagrams.

References

Braun, P. B. & Vucht, J. H. N. v. (1955). *Acta Cryst.* **8**, 117.
Nowotny, H. (1942). *Z. Metallk.* **34**, 23.

Notes and News

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