and equation (1) reduces to

$$B_{\mathbf{h}}^{\text{n.s.}} = \frac{|F_{\mathbf{h}}|^2 - |F_{-\mathbf{h}}|^2}{4f_a'} \ . \tag{5}$$

The criteria for optimum wavelengths for phase determination are found in the denominators of equations (4) and (5); first, that one radiation gives a large value of the out-of-phase component $f_a^{\prime\prime}$, for one or more atoms, which will give a large difference in the observed reflections $F_{\mathbf{h}}^2$ and $F_{-\mathbf{h}}^2$; secondly, that the difference of the in-phase components of anomalous scattering for the two radiations, $(\Delta f_{a\lambda_1}^{\prime} - \Delta f_{a\lambda_2}^{\prime})$, be as large as possible to produce a large difference in the observed mean square values $\mathcal{F}_{\mathbf{h}\lambda}^2$ and $\mathcal{F}_{\mathbf{h}\lambda}^2$.

The accuracy of the method is dependent upon an exact knowledge of the anomalous scattering increments

 $\Delta f'$ and f'' to the atomic scattering factor. The table of these values calculated by Dauben & Templeton (1955) for $Z\gtrsim 20$ is for three radiations ${\rm Cr}\ K\alpha$, ${\rm Cu}\ K\alpha$ and Mo $K\alpha$ only. Values for intermediate radiations can be estimated by interpolation, but for general application of this method of calculation of exact values, or their experimental measurement, a full range of radiations would be of great assistance.

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Acta Cryst. (1957). 10, 476

The crystal structures of thorium bismuthides. By Riccardo Ferro, Chemical Institute, Laboratory of Physical Chemistry of Genoa University, Genoa, Italy

(Received 3 April 1957)

The diagram of the thorium-bismuth alloys, obtained in vacuo by direct synthesis from the elements, has been studied by means of X-rays; the examination was performed by the powder method using $Cu K\alpha$ radiation $(\lambda(Cu K\alpha_1) = 1.540500 \text{ Å})$. The only impurity in the thorium used (prepared by reduction of ThO₂ with Ca) was about 0.3% oxygen, mainly as ThO₂; the bismuth had a purity higher than 99.9%, with traces of lead.

In the part of the diagram richer in bismuth the alloys show the existence of the compounds Th₃Bi₄ and ThBi₂. No other compounds having higher quantities of bismuth have been observed, as alloys of a composition of around 80% Bi (both quenched from 1000° C. or annealed up to 400° C.) showed only the Debye reflexions of ThBi₂ and elementary bismuth.

The X-ray examination of the central part of the diagram shows the possible existence of two phases of a composition near to ThBi; however, it was not possible (with several thermal treatments, including also annealing and heating to higher temperatures) to obtain a cubic phase of the NaCl- or CsCl-type, as might expected by comparison with similar systems of thorium and uranium with other metalloids. With regard to these alloys it must be remarked that, if heated *in vacuo* at approximately 1500° C., they undergo alteration by bismuth distillation.

Finally, the alloys with a low bismuth content have not shown (after heating at a high temperature and cooling) the formation of other compounds: samples which on analysis had a composition around 30% Bi show mainly the reflexions of elementary thorium.

As with bismuth and the intermediary phases, the photographs exclude the formation of appreciable solid solution for thorium. All the alloys are fairly pyrophoric.

Th₃Bi₄

The compound Th₃Bi₄ (45·44% Th) is body-centred cubic with

$$a_0 = 9.559 \text{ Å}, Z = 4, \varrho = 11.65 \text{ g.cm.}^{-3}.$$

The structure is of the Th_3P_4 type (Meisel, 1939), $D7_3$ type (Strukturbericht, 1943) with:

Space group No. 220 (International Tables, 1952): I43d.

Atomic positions:

12 Th in (a)
$$(0, 0, 0; \frac{1}{2}, \frac{1}{2}, \frac{1}{2}) + \frac{3}{8}, 0, \frac{1}{4}; \mathbb{Q}$$
.
16 Bi in (c) $(0, 0, 0; \frac{1}{2}, \frac{1}{2}, \frac{1}{2}) + x, x, x;$
 \mathbb{Q} with $x = \frac{1}{12}$.

Each thorium atom is thus bound to 8 bismuth atoms at the distance of 3.32 Å.

ThBi₂

The compound ThBi₂ (35.70% Th) is tetragonal with

$$a_1 = 4.492, \ a_3 = 9.298 \text{ Å}, \ a_3/a_1 = 2.070, \ Z = 2, \ \varrho = 11.50 \text{ g.cm.}^{-3}.$$

The structure corresponds to the C38 type (Strukturbericht, 1937) with:

Space group No. 129 (International Tables, 1952): P4/nmm.

Atomic positions:

2 Bi_I in (a) 0, 0, 0;
$$\frac{1}{2}$$
, $\frac{1}{2}$, 0.

2 Bi_{II} in (c)
$$0, \frac{1}{2}, x; \frac{1}{2}, 0, \overline{x}$$
 with $x = 0.63$.

2 Th in (c')
$$0, \frac{1}{2}, t; \frac{1}{2}, 0, \bar{t}$$
 with $t = 0.28$.

The Th-Bi distances are:

Th-4 Bi_{II} = 3.44; Th-1 Bi_{II} = 3.26; Th-4 Bi_{II} = 3.29 Å. The smallest Bi-Bi distance is Bi_I-4 Bi_I = 3·18 Å.

The above mentioned compounds are isostructural with both U3Bi4 and UBi2 (Ferro, 1952, 1953) and with Th₃As₄, ThAs₂ (Ferro, 1955) and Th₃Sb₄, ThSb₂ (Ferro, 1956) previously studied.

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Acta Cryst. (1957). 10, 477

Elementarzelle des cyclischen Nylon-Oligomeren 1,8,15,22-tetra-aza-2,7,16,21-tetra-oxocyclo-octacosan. Von Hans von Dietrich, Helmut Zahn* und Franz Schmidt, Chemisches Institut der Universität Heidelberg, Deutschland

(Eingegangen am 11. März 1957)

$$\begin{array}{cccc} O & O \\ || & || \\ NH-C-(CH_2)_4-C-NH \\ | & | \\ (CH_2)_6 & (CH_2)_6 \\ || & | \\ NH-C-(CH_2)_4-C-NH \\ || & || \\ O & O \\ (I) \end{array}$$

kristallisiert aus Wasser in monoklinen Blättchen (Zahn et al., 1956a; Brown, Hill & Youle, 1956; Zahn, Miro & Schmidt, 1957); Blättchenebene (010), Spaltbarkeit nach (001) angedeutet.

Die röntgenographische Untersuchung ergab folgende Daten:

Das aus Nylon 66 isolierbare cyclische Oligomere (I) $a_0 = 10.78 \pm 0.03$, $b_0 = 25.12 \pm 0.05$, $c_0 = 9.67 \pm 0.02$ Å, $\beta = 92^{\circ} 22' \pm 6'$.

Nimmt man an, dass die Zelle vier Moleküle enthält, so ergibt sich die Dichte = $1,149\pm0,005$ g.cm.⁻³ (bei 25-27° C.). Gemessen wurde: 1,148 g.cm.-3 (bei 28° C.).

Der aus Debye-Scherrer-Aufnahmen bestimmte Netzebenenabstand von 12,6 Å (Schmidt, 1956; Zahn et al., 1956b), also gerade $\frac{1}{2}b_0$, lässt darauf schliessen, dass die Ausdehnung der Einzelmoleküle auch in Richtung der b-Achse höchstens 12,6 Å ist, was in Verbindung mit den übrigen Abmessungen der Elementarzelle eine starke Faltung der Ringe fordert. Bei völliger Streckung der Einzelmoleküle haben diese eine Länge von ca. 20 Å.

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A graphical method for the calculation of $|F|^2$ and |F| from equi-inclination Weissenberg photographs. By Kurt Boström, Department of Mineralogy, Swedish Museum of Natural History, Stockholm 50, Sweden (Received 2 April 1957)

Introduction

In a given Weissenberg equi-inclination photograph the intensities of the spots obey the equation

$$I = C.\lambda^3.A \frac{1 + \cos^2 2\theta}{\cos^2 \mu \sin \nu}.|F|^2 \tag{1}$$

if the extinction is not taken into consideration. Here C is constant and A an absorption factor. The other symbols are identical with those used by Buerger (1942).

We can write (1) in the following way:

$$|F|^2 = \frac{I}{C \cdot \lambda^3 \cdot A} \cdot \frac{\cos^2 \mu \cdot \sin \gamma}{1 + \cos^2 2\theta}.$$
 (2)

Lu (1943) introduced the abbreviation

$$\alpha = \frac{\cos^2 \mu \cdot \sin \gamma}{1 + \cos^2 2\theta} \,. \tag{3}$$

If $C.\lambda^3.A = 1$, equation (1) becomes

$$|F|^2 = I \cdot \alpha . \tag{4}$$

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