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The crystal structure of Sc_3In.

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Ferromagnetism in the scandium–indium system is being investigated by Matthias, Clogston, Williams, Corenzwit & Sherwood (1961). The crystal structure of the compound Sc_3In is reported here.

An ingot was prepared by reacting Sc and In in the proportions 3·15 to 1 in an arc furnace under an argon atmosphere and then annealing the sample at 800 °C. for one week. X-ray diffraction photographs were taken of the resulting product using a Norelco camera of 114·6 mm. diameter and Cu K-radiation ($\lambda = 1{\cdot}5418$ Å). The pattern resembled that of scandium with somewhat smaller lattice constants. However, the presence of some extra lines suggested the possibility of a superlattice. To investigate this, filings of the melt were annealed at 390 °C. for two weeks. The powder diffraction pattern of this material could be indexed on a hexagonal lattice with

$$a = 6{\cdot}421 \pm 0{\cdot}005,\ c = 5{\cdot}183 \pm 0{\cdot}005\ \text{Å}\ .$$

The observed and calculated interplanar spacings are listed in Table 1. There are two extremely weak extra lines which are probably due to another phase in the Sc–In system.

Table 1. *Comparison of observed and calculated interplanar spacings and intensities*

hk·l	d_o	d_c	I_o*	I_c
10·0	5·539 Å	5·561 Å	*m*	100
10·1	3·770	3·791	*s*	244
11·0	3·187	3·211	*m*	108
20·0	2·763	2·780	*vs*	245
00·2	2·585	2·592	*vs*	265
20·1	2·449	2·450	*vvs*	1000
11·2	2·010	2·017	*w*	61
21·1	1·945	1·948	*w–m*	83
20·2	1·888	1·896	*m–s*	150
22·0	1·603	1·605	*m–s*	166
31·1	1·475	1·478	*vvw*	34
20·3	1·463	1·467	*s*	183
22·2	1·361	1·365	*s*	191
40·1	1·341	1·343	*m–s*	136
40·2	1·222	1·225	*vw*	33
40·3	1·082	1·083	*w–m*	72
42·1	1·029	1·030	*m–s*	127
22·4	1·008	1·008	*m*	85
42·2	0·9710	0·9739	*m*	42
20·5		0·9713		61
60·0	0·9271	0·9268	*vw* (diffuse)	42
42·3	0·8973	0·8978	*m–s*	127
60·2	0·8726	0·8727	*m*	91
40·5	0·8317	0·8311	*m*	84
42·4	0·8169	0·8162	*w–m*	64

* Visually estimated

(*vs* = very strong; *s* = strong; *m* = medium; *w* = weak).

To conserve space, calculated intensities below 30 are omitted.

Relative intensities were calculated based on a Mg_3Cd type structure (DO_{19}) which is a superlattice derived from hexagonal close-packing (Wells, 1950). The presence of a superlattice was suggested by the fact that the axial length a is approximately twice that of Sc.

The Mg_3Cd structure was determined by Dehlinger (1930). The space group is D_{6h}^4–$P6_3/mmc$ with two formula weights per unit cell. The atom positions are:

$$6\,\text{Sc in } (h);\ x, 2x, \tfrac{1}{4};\ 2\bar{x}, \bar{x}, \tfrac{1}{4};\ x, \bar{x}, \tfrac{1}{4};\ \bar{x}, 2\bar{x}, \tfrac{3}{4};\ 2x, x, \tfrac{3}{4};\ \bar{x}, x, \tfrac{3}{4};\ x = \tfrac{5}{6}.$$

$$2\,\text{In in } (c);\ \tfrac{1}{3}, \tfrac{2}{3}, \tfrac{1}{4};\ \tfrac{2}{3}, \tfrac{1}{3}, \tfrac{3}{4}.$$

The intensities were computed for $x = 0{\cdot}823$, 0·833 and 0·843. The best agreement between calculated and observed intensities, visually estimated, is obtained for $x = 0{\cdot}833$. The results are given in Table 1. The low intensity of the low angle lines is probably due to absorption. Satisfactory agreement between the observed and calculated intensities confirmed the Mg_3Cd type structure for Sc_3In.

The structure consists of 4 A3 type (h.c.p.) unit cells in which $\frac{1}{4}$ of the Sc atoms are replaced by In. In this structure the nearest neighbors to an In atom are 12 Sc atoms at approximately 3·20 Å. The Sc atom is surrounded by 4 In atoms at approximately 3·20 Å and 8 Sc atoms at about 3·20 Å.

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Unit cell and space group of mercury tellurate, Hg_3TeO_6.

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Because of its cubic symmetry and its large unit cell mercury tellurate is well suited as an internal standard material for high accuracy X-ray powder analysis. It may be prepared according to Hutchins (1905) by reaction between concentrated aqueous solutions of potassium tellurate and mercury nitrate in a weakly acid solution.