

Acta Cryst. (1962). **15**, 1062

A new hexagonal phase between Au_4Mn and Au_3Mn . By D. P. MORRIS and J. L. HUGHES, *Physics Department, University College of North Wales, Bangor, Wales*

(Received 15 March 1962 and in revised form 16 May 1962)

In the course of a study of the gold-manganese equilibrium diagram a new hexagonal η phase has been observed in the region between Au_4Mn and Au_3Mn . It has a very narrow range of homogeneity and has not been observed entirely as a pure phase. We have established that it is centred very near to 23.8 at.% Mn and exists up to about 620 °C. above which temperature it reverts to the α f.c.c. solid solution of manganese in gold.

Alloy samples have been examined both in a high-

Table 1. Data for the η phase in alloy 23.6

hkl	d_o	d_c	I_o	I_c
10·0	2.465 Å	2.477 Å	mw	8
00·2	2.357	2.367	m*	37
10·1	2.186	2.195	vs	100
10·2	1.706	1.711	w	5
11·0	1.426	1.413	ms	22
10·3	1.3273	1.3312	m	20
20·0	1.2388	1.2375	vw	0.9
11·2	1.2212	1.2230	ms	27
20·1	1.1952	1.1972	mw	14
00·4	1.1807	1.1824	w	3.7
20·2	1.0963	1.0964	vw	1.2
10·4	1.0666	1.0669	vw	1.2
20·3	0.97306	0.97343	mw	9.6
21·1	0.91762	0.91807	m	19.5
11·4	0.91091	0.90992	m	17.4
10·5	0.88350	0.88360	mw	9.6
21·2	0.87048	0.86987	w	2.4
20·4	0.85471	0.85490	vw	1.3
30·0	0.82461	0.82499	vw	0.8
21·3	0.80448	0.80449	s	36
00·6	0.78818	0.78829	mw	7
30·2	0.77900	0.77895	s	61

$\lambda_{\alpha_1} = 1.54051 \text{ \AA}$ for reflections above 11·0; $\lambda_{wm} = 1.54178 \text{ \AA}$ below 11·0.

I_o = visually estimated intensity (*vs* = very strong; *s* = strong; *m* = medium; *w* = weak).

* The 00·2 line was near to the 111 line of the orthorhombic α'' structure mentioned in the text.

I_c = calculated intensity for a 'mean atom' of atomic number 66. No correction for absorption and temperature was applied.

Density of alloy = M 16 g.cm.⁻³. Theoretical density for *A3* structure = 16.16 g.cm.⁻³.

temperature X-ray camera and in a quenched condition. The data given in Table 1 was obtained from a powder sample of alloy 23.6,* which was quenched after three days at 490 °C. and photographed at room temperature using $\text{Cu K}\alpha$ radiation. This enabled the structure to be identified as hexagonal, the cell dimensions determined by Cohen's method being:

$$a = 2.8578 \pm 0.0003, c = 4.7297 \pm 0.0003 \text{ \AA}, \\ c/a = 1.6550, \text{ at } 22 \text{ }^\circ\text{C}.$$

The calculated intensities I_c shown in the table are in agreement with the *A3* type of structure with the gold and manganese at random in the hexagonal lattice.

Between the η phase and the tetragonal α' structure of Au_4Mn (Kussmann & Raub, 1956; Watanabe, 1960a) there exists an orthorhombic structure α'' . A small amount of this phase occurred in the sample of Table 1. α'' was found as a pure phase between about 21.0 and 22.2 at.% Mn after appropriate heat treatment. In alloy 21.0 quenched from 445 °C. the lattice parameters of its fundamental cell are

$$a = 4.0814 \pm 0.0003, b = 4.0599 \pm 0.0003, \\ c = 4.0377 \pm 0.0003 \text{ \AA}.$$

α'' changes to tetragonal α' in this alloy below about 400 °C., in which state it is ferromagnetic at room temperature. In alloy 24.0 η coexisted with a complex structure, presumably Au_3Mn (Watanabe, 1960b).

A detailed account of the equilibrium diagram in this region will be published elsewhere.

We wish to thank the Council of the Royal Society for a grant-in-aid, and the D.S.I.R. for a maintenance grant to one of us (J. L. H.).

References

- KUSSMANN, A. & RAUB, E. (1956). *Z. Metallk.* **47**, 9.
WATANABE, D. (1960a). *J. Phys. Soc., Japan*, **15**, (7), 1251.
WATANABE, D. (1960b). *J. Phys. Soc., Japan*, **15**, (6), 1030.

* Alloy 23.6 means an alloy of composition 23.6 at.% Mn.

Acta Cryst. (1962). **15**, 1062

Kristallographische Daten des Selenocarbohydrazids, $\text{CSe}(\text{NH}-\text{NH}_2)_2$. Von F. FEHÉR, D. HIRSCHFELD und K.-H. LINKE, *Institut für Anorganische Chemie der Universität Köln, Deutschland*

(Eingegangen am 13. Juni 1962)

Aus Drehkristall-, Goniometer- und Retigraphenaufnahmen um die verschiedenen Achsen eines aus wässriger Lösung gewonnenen Kristalls ergaben sich für die Gitterkonstanten des monoklin kristallisierenden Selenocarbohydrazids (Fehér *et al.*) folgende Werte:

$$a = 6.16, b = 15.50, c = 4.81 \text{ \AA}; \beta = 96^\circ 59'.$$

Die Elementarzelle ist mit 4 Molekülen Selenocarbohydrazid besetzt, die Dichte lässt sich danach zu 2.216 g.cm.⁻³ berechnen.

Aus den Auslöschungen folgen für diese Verbindung die Raumgruppen $C_2^2-P2_1$ und $C_{2h}^2-P2_1/m$.

Aufgrund von Modellbetrachtungen ergibt sich unter Berücksichtigung einer möglichst guten Raumerfüllung ein recht plausibler Strukturvorschlag, der z.Zt. noch durch Intensitätsmessungen geprüft wird.

Literatur

- FEHÉR, F., HIRSCHFELD, D. & LINKE, K.-H. (1962). *Z. Naturforsch.* (Im Druck.)