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Errata in *International Tables for X-ray Crystallography*, Vol. I (2nd edition).

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A corrected electron density expression is given for space groups $P4_122$ (No. 91) and $P4_322$ (No. 95).

The electron density expressions for the enantiomorphous space groups $P4_122$ (No. 91, p. 426) and $P4_322$ (No. 95, p. 429) should read:

$$\varrho(XYZ) = \frac{8}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{l=2n}|F(hkl)|\,[\cos 2\pi hX \times \cos 2\pi kY \cos 2\pi lZ \cos\alpha(hkl) - \sin 2\pi hX \sin 2\pi kY \sin 2\pi lZ \sin\alpha(hkl)] + \sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{l=2n+1}|F(hkl)|\,[-\sin 2\pi hX \times \cos 2\pi kY \sin 2\pi lZ \cos\alpha(hkl) + \cos 2\pi hX \sin 2\pi kY \cos 2\pi lZ \sin\alpha(hkl)]\right\}.$$

Corrections to the phase relationships have appeared already (Schultze-Rhonhof, 1966).

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The structure of Mn_2Au and Mn_3Au.

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X-ray and neutron diffraction measurements have shown that Mn_2Au is a compound with a tetragonal unit-cell of dimensions $a=3{\cdot}328$ and $c=8{\cdot}539$ Å and that it can be assigned to the same space group as $MnAu_2$, namely $I4/mmm$ ($D_{4h}{}^{17}$). The neutron diffraction pattern of 74·2 at.% MnAu can be explained only if the ordered structure of this alloy is identical with that of Mn_2Au. Thus the compound Mn_3Au apparently does not exist.

Introduction

In their investigation of the phase diagram of the Mn–Au system, Raub, Zwicker & Baur (1953) proposed the existence of the compound Mn_3Au, and from X-ray diffraction of a 70 at. % Mn alloy they concluded that it had a complex tetragonal structure, and also remarked on the similarity of the diffraction pattern to that obtained from an alloy of composition Mn_2Au.

Gaunt & Eden (1965) proposed a tetragonal structure for Mn_3Au with cell dimensions $a=4{\cdot}706$, $c=8{\cdot}539$ Å and atomic coordinates

Au: 000; $\frac{1}{2}0\frac{1}{2}$; $0\frac{1}{2}\frac{1}{2}$;
Mn: $00\pm z$; $\frac{1}{2}0\frac{1}{2}\pm z$; $0\frac{1}{2}\frac{1}{2}\pm z$
$\frac{1}{2}\frac{1}{2}\pm z$; $\frac{1}{2}\frac{1}{2}0$

with $z\simeq\frac{1}{3}$.

They also commented on the close similarity of this structure to that determined for $MnAu_2$ by Hall & Royan (1959).

During an investigation of Mn_3Au it was found that the neutron diffraction patterns could not be explained in terms of the above structure, and this prompted the following study.

Experimental

Three ingots, each weighing about 60g, were prepared by melting together manganese (4*N*5) and gold (5*N*) in an argon arc furnace. The ingots were homogenized at 900 °C *in vacuo* for 50 hours and annealed at 500 °C for a further 50 hours. Chemical analysis showed the compositions of the ingots to be 62·6, 67·4 and 74·2 at. % Mn.

X-ray diffraction patterns from flat polished specimens of all three compositions were similar to that reported by