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The Crystal Structure of Ti_3Au and Ti_3Pt

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Powder patterns indicate that Ti_3Au and Ti_3Pt crystallize in the $A15$ (β-wolfram) structure with lattice parameters of 5·096 and 5·033 Å, respectively.

An exploratory X-ray investigation of the titanium–gold and titanium–platinum systems revealed the presence of intermediate phases in the vicinity of the compositions Ti_3Au and Ti_3Pt. The crystal structures of these new phases were worked out from powder patterns and are described in the present note.

The alloys were prepared by rolling suitable amounts of the constituent metals into thin flat strips, which were then wrapped together and arc melted in an atmosphere of high-purity helium by a technique which has been described elsewhere (Schramm, Gordon & Kaufmann, 1950). The gold and platinum were 'commercially pure' grade (i.e. at least 99·9% pure) and the titanium (prepared by the iodide decomposition process) contained less than 0·05% total impurities by the vendor's analysis.

After arc melting, the Ti_3Au specimen was sealed in an evacuated silica tube and heated for 75 hr. at 1500° F. The Ti_3Pt specimen was not given any further heat treatment. Both specimens were crushed, and portions of the resulting powders which passed through a 200 mesh screen were used to obtain X-ray diffraction patterns with a camera of 14·32 cm. diameter and copper $K\alpha_1$ radiation.

The powder patterns thus obtained were easily indexed as those of simple cubic lattices having parameters of 5·096 Å for the Ti_3Au and 5·033 Å for the Ti_3Pt. These values of the parameters were computed by applying Cohen's (1935) least-squares method to the last ten back-reflection lines of each pattern. The possibility that the structure of these compounds (which the powder patterns showed at once to be isomorphous) is the $A15$ or β-wolfram structure was suggested by the AB_3 atomic ratio, by the positions of the constituent metals in the periodic table, and by the fact that reflections of the type (hhl) with odd l are missing, as required by the space group O_h^3 of the $A15$ structure. Accordingly, relative intensities were computed by the formula

$$I \propto p|F|^2 \frac{1+\cos^2 2\theta}{\sin^2\theta \cos\theta},$$

where p is the planar multiplicity factor, F is the structure factor, and the angular factor represents the

Table 1. *Diffraction data for* Ti_3Au

	I_o		
hkl	Film	Spectrometer	I_c
110	*w*	630	764
200	*w*	520	424
210	*vw*	250	192
211	*m*	1000	1000
220	*vw*	150	118
310	*w*	200	165
222	—	—	8
320	*vw*	60	36
321	*ms*	640	475
400	*w*	150	87
411, 330	*w*	140	97
420	*mw*	170	137
421	*vvw*	—	8
332	*mw*	—	123
422	*vw*	—	47
510, 431	*mw*	—	136
520, 432	*vw*	—	39
521	*m*	—	215
440	*mw*	—	103
530, 433	*mw*	—	104
600, 442	*m*	—	168
610	*vvw*	—	17
611, 532	*s*	—	460
620	*vw*	—	84
541	*m*	—	258

s=strong; *ms*=medium strong; *m*=medium; *mw*=medium weak; *w*=weak; *vw*=very weak; *vvw*=very very weak.

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Table 2. *Diffraction data for* Ti_3Pt

	I_o		
hkl	Film	Spectrometer	I_c
110	*w*	550	749
200	*w*	470	424
210	*vw*	250	199
211	*ms*	1000	1000
220	*vw*	130	116
310	*w*	190	165
222	—	—	7
320	*vw*	70	36
321	*ms*	590	474
400	*vw*	100	89
411, 330	*w*	150	96
420	*w*	150	138
421	*vvw*	—	8
332	*w*	—	123
422	*vw*	—	46
510, 431	*mw*	—	132
520, 432	*vw*	—	40
521	*ms*	—	217
440	*mw*	—	104
530, 433	*mw*	—	102
600, 442	*m*	—	169
610	*vvvw*	—	17
611, 532	*s*	—	464
620	*vw*	—	83
541	*m*	—	258

s=strong; *ms*=medium strong; *m*=medium; *mw*=medium weak; *w*=weak; *vw*=very weak; *vvw*=very very weak.

combined Lorentz and polarization factors. Table 1 lists the relative intensities. The agreement is satisfactory except for the reflections of low Bragg angles. It was felt that this discrepancy was due to the large absorption of the gold and platinum atoms. In order to check this hypothesis, a pattern of each substance was taken on a Norelco spectrometer. Since in this apparatus all lines of the pattern are obtained by Bragg-type reflection rather than by Laue-type, effects due to absorption in the low-angle reflections should be considerably less than in the case of a pattern obtained photographically. The relative intensities (above local backgrounds) measured on the Norelco charts are given in Table 1, and it can be seen that those of the lowest-angle reflections are indeed in much better agreement with the calculated values than are those read from the films.

The structures proposed on the basis of these results are accordingly as follows:

Space group O_h^3–$Pm3n$; 8 atoms per unit cell.
$a_0 = 5{\cdot}096$ Å for Ti_3Au; $= 5{\cdot}033$ Å for Ti_3Pt.
2 Au (or Pt) atoms in (*a*): $0, 0, 0$; $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$.
6 Ti atoms in (*d*): $\frac{1}{4}, \frac{1}{2}, 0$; $0, \frac{1}{4}, \frac{1}{2}$; $\frac{1}{2}, 0, \frac{1}{4}$; $\frac{3}{4}, \frac{1}{2}, 0$; $0, \frac{3}{4}, \frac{1}{2}$; $\frac{1}{2}, 0, \frac{3}{4}$.

In Ti_3Au, each gold atom is surrounded by twelve titanium atoms at a distance of 2·84 Å; each titanium atom is surrounded by two titanium atoms at 2·54 Å, four gold atoms at 2·84 Å, and eight titanium atoms at 3·11 Å. In Ti_3Pt, each platinum atom is surrounded by twelve titanium atoms at 2·81 Å; each titanium atom is surrounded by two titanium atoms at 2·51 Å, four platinum atoms at 2·81 Å, and eight titanium atoms at 3·07 Å.

As a result of a literature survey, it appears that the following intermetallic phases also crystallize in the β-wolfram structure: Cr_3Si (Boren, 1933), V_3Si (Wallbaum, 1939), Cr_3Ge and V_3Ge (Wallbaum, 1944), Mo_3Si (Templeton & Dauben, 1950), and V_3Co (Duwez, 1951). The fact that Mo_3Zr also has the β-wolfram structure has been reported by Wallbaum (1942). An X-ray investigation of the molybdenum–zirconium system in this laboratory indicates that the only intermediate phase in this system is centered around Mo_2Zr and that its structure is not that of β-wolfram.

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