

(Borie, 1956) and $A = 63.5$. Then J is about one-eighth of the average room temperature TDS and nearly half at 80 °K. Near the edges of a Brillouin zone (where in the case of short range order the diffuse scattering of interest is usually concentrated) J is a larger fraction of the TDS, and near the fundamental Bragg maxima it is a smaller part of the total correction. For measurements made in the usual low angle range ($2\theta = 20^\circ - 40^\circ$) with Cu $K\alpha$ radiation, J is roughly an order of magnitude greater than the second order TDS at room temperature.

For most of the diffuse scattering experiments listed in the references, the correction discussed here would be small and perhaps unimportant. It is likely to be useful in future high precision measurements made either

on dilute solid solutions or those with a small difference in the atomic scattering factors of the two components.

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The influence of impurities on the formation of the Cu_3Au -type structure from the Cr_3Si -type structure. By HENNING VON PHILIPSBORN and F. LAVES, *Institute of Crystallography, Swiss Federal Institute of Technology, Zürich, Switzerland*

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The intermetallic compounds Ti_3Au (Duwez & Jordan, 1952), V_3Au (Wood & Matthias, 1956), and V_3Pt (Greenfield & Beck, 1956), are known to have the Cr_3Si ($A15$)-type structure.* In this investigation stoichiometric amounts of the respective elements were melted or, alternatively, the single-phase compounds were remelted in an argon-arc furnace, a water-cooled copper crucible being used. In the presence of small amounts of oxygen, nitrogen, or carbon, we obtained, along with the Cr_3Si -type structure (hereafter called β phase), a second phase having the ordered Cu_3Au ($L1_2$)-type structure (hereafter called α phase). The amount of α phase formed depends upon the purity of the titanium (99.9% Johnson & Matthey, and less pure from other sources), and vanadium (99.8% Union Carbide, and less pure from other sources) used, and upon the amount of oxygen, nitrogen or carbon picked up during melting. Titanium and vanadium are known to contain oxygen and nitrogen as main impurities.

Melting losses under pure argon (200 Torr, 10^4 cm^3) were about 0.1 wt.% for Ti_3Au (weight of charge 1–4 g). Thus a weight increase by melting in the presence of oxygen or nitrogen indicates the amount picked up during melting. This amount was controlled by variation of the melting time. Remelting $\beta \text{Ti}_3\text{Au}$, e.g. for 10 sec in the presence of oxygen (15 Torr), resulted in the pickup of about 1 wt.% (4.5 at.%) oxygen and the formation of about 40% α phase. Introducing the oxygen by premelting the titanium with TiO yielded the same results. Total conversion of β to $\alpha \text{Ti}_3\text{Au}$ was obtained for 3.4 wt.% (16 at.%) oxygen. Nitrogen and carbon have about the same influence, hydrogen none. V_3Au needs much less oxygen (about 0.7 wt.% or 3 at.%) for complete transformation.

The transformation is irreversible. No β phase was

restored when $\alpha \text{Ti}_3\text{Au}$ created by oxygen was remelted in an electron beam furnace under high vacuum (5×10^{-7} Torr) for 2×10 min. Annealing at 400 °C to 1200 °C for up to 40 days and rapid quenching had no effect. The two phases of Ti_3Au were present within the same range $\text{Ti}_{85}\text{Au}_{15}$ to $\text{Ti}_{85}\text{Au}_{15}$. Melting 50/50 mixtures of V_3Pt with Ti_3Au , Nb_3Au , and Nb_3Pt results in mixtures of the α and β phases with intermediate lattice constants.

Micrographs of Ti_3Au specimens containing 10–20% α phase, according to X-ray determination, revealed regularly oriented dendrites 5–10 μ in diameter. Small dendrite-rich regions of the specimens showed more α phase in X-ray pattern than dendrite-poor regions, indicating that the dendrites are α phase. Dr Kurt F. J. Heinrich kindly examined the specimens by electron microprobe analysis: 'The acicular inclusions have lower electron backscatter and higher target current than the surroundings. Emitted characteristic X-ray lines of both Ti and Au show lower intensities within the inclusions than in the matrix. These results would indicate that an element of low atomic number should be present, at rather low concentrations, in this particular phase' (Heinrich, 1963).

Table 1 shows lattice constants of α phases found. The lattice constants of the β phases agree well with the values given in the literature. The X-ray density of the β phase is from 6–9% larger than that of the α phase. Table 2 shows the good agreement between

Table 1. Lattice constants of α and β phases and ratio of X-ray densities β/α

Compound	α Phase created by	Lattice constant $\pm 0.002 \text{ \AA}$		Ratio of X-ray densities
		α phase	β phase	
Ti_3Au	O, N	4.096	5.096	1.063
Ti_3Au	C	4.147	5.096	1.078
V_3Au	O, N	3.964	4.876	1.074
V_3Pt	?	3.932	4.817	1.088
V_3Pt	O	3.918	4.817	1.076

* Cr_3Si (Borén, 1933) was the first compound definitely shown to have the ($A15$) structure. According to Hägg & Schönberg (1954) W_3O (β tungsten) is completely disordered and according to Kihlberg (1962), the existence of Cr_3O recently used to designate the ($A15$) structure is not confirmed.

Table 2. Comparison of observed and calculated intensities of the α phase of Ti_3Au and V_3Au , neglecting impurity (O, N, C) contents

<i>hkl</i>	αTi_3Au		αV_3Au	
	I_o	I_c	I_o	I_c
100	41	55	36	52
110	48	48	52	45
111	100	100	100	100
200	43	48	64*	48
210	26	25	25	24
211	27	20	26	19
220	40	31	41	30
221, 300	18	13	14	14
310	13	9	12	8
311	33	36	42	36
222	10	11	14	11

* This reflexion might be reinforced by the presence of some residual β phase the strongest reflexion of which, 211, coincides with 200 of the α phase.

the observed and calculated intensities of the α phases of Ti_3Au and V_3Au and indicates the correctness of the proposed structure. Intensities were measured with an X-ray powder diffractometer and calculated according to the formula $I \sim p|F_{hkl}|^2(1 + \cos^2 2\theta)/(\sin^2 \theta \cos \theta)$.

Our observations explain discrepancies in the literature. Laves & Wallbaum (1939) reported Ti_3Au to have the Cu_3Au -type structure, which was not confirmed by: Duwez & Jordan (1952), Pietrokowsky, Frink & Duwez (1956), Stolz & Schubert (1962). Probably the titanium available in 1939 contained enough impurities to suppress the formation of βTi_3Au . For V_3Au Wood & Matthias (1956) mention the existence of two 'very very weak' extra lines. The d values were 2.28 and 1.44 Å. Their origin was left unexplained. $d = 2.28$ Å corresponds exactly to the strongest reflexions of αV_3Au .

Impurity stabilization of special structure types is well known. Stadelmaier (1961) examined ternary phases of T -metals (Mn, Fe, Co, Ni, Pd, Pt), B -metals (Mg, Zn, Cd, Hg, Al, Ga, Ge, In, Sn, Pb), and metalloids (B, C, N).

He found that the Cu_3Au -type structure could be stabilized by carbon and nitrogen and proposed that the metalloid partly fills the octahedral hole of the ($L1_2$) structure, yielding perovskite-type structures in extreme cases.

For αTi_3Au , the radius of the octahedral hole equals 0.60 Å, which agrees well with a radius of the O atom (0.60 Å) as shown by Ehrlich (1941) for solutions of oxygen in metallic titanium. That in the Cu_3Au -type structure the O occupies the central octahedral hole is also supported by detailed intensity discussions to be published elsewhere.

We thank Dr Kurt F. J. Heinrich of E. I. du Pont de Nemours and Co., Pigments Department, Wilmington and Mr Z. de Beer of Applied Research Laboratories, Lausanne for performing the electron microprobe experiments on the Ti_3Au specimens and Dr E. Bucher of Physics Institute ETH for performing the melting experiments in the electron beam furnace.

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Notes and News

Announcements and other items of crystallographic interest will be published under this heading at the discretion of the Editorial Board. The notes (in duplicate) should be sent to the General Secretary of the International Union of Crystallography (D. W. Smits, Mathematisch Instituut, University of Groningen, Reithdiepskade 4, Groningen, The Netherlands). Publication of an item in a particular issue cannot be guaranteed unless the draft is received 8 weeks before the date of publication.

International Union of Crystallography Acta Crystallographica

The Executive Committee of the Union and the Commission on *Acta Crystallographica* regret to announce the resignation of Professor I. Nitta as Co-editor of *Acta Crystallographica*. Professor Nitta was appointed in 1952, to aid in the editing of papers originating in Japan and its neighbourhood, and the Union is greatly indebted to him for his work in this field and his wise counsel on other matters.

The Executive Committee has approved the appointment of Professor S. Miyake, of the Institute for Solid State Physics of the University of Tokyo, as successor to Professor Nitta.

Symposium on OD-Structures and Related Problems

A symposium on OD-structures; Structure and twinning; and Superstructures and substructures; is being organized by the Slovenská Akadémia Vied and the Deutsche Akademie der Wissenschaften zu Berlin. The symposium will take place in Smolenice, Czechoslovakia, from 19 to 23 May 1964, and will be limited to about 35 participants. Further information may be obtained from Professor K. Boll-Dornberger, Institut für Strukturforchung DAW, Rudower Chaussee, Berlin-Adlershof, Germany.