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INTERSTITIAL ORDERING IN TANTALUM

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In recent years, there have been a number of investigations of the structure of interstitially ordered phases obtained as a result of the introduction of itnerstitials into the Group V B body centered cubic metals [1-8]. Of particular interest is the structure of the interstitially ordered phase obtained on the introduction of carbon into tantalum.[1,7,8]

Villagrana and Thomas [1] have shown that Ta-C alloys containing up to three atomic percent carbon are ordered. On the basis of electron diffraction data, the existence of a new phase, $Ta_{64}C$, was predicted (see Figs. 6 and 7 of ref. 1). The existence of this ordered phase, corresponding to a chemical composition of 1.56 atomic percent carbon, has been confirmed in a recent investigation [7] and the effect of the microstructural changes accompanying this interstitial ordering transformation on the mechanical properties of tantalum-carbon alloys will be reported later.[8]

Since the results of Villagrana and Thomas have been published, identical electron diffraction patterns to those from $Ta_{64}C$ have been reproted for vanadium-oxygen alloys [3] and re-interpreted in terms of the $V_{64}O$ structure.[2] More recently Steeb and Renner[4] and Geiss and Lawless[6] working on the Ta-O system also obtained identical results to those of $Ta_{64}C$ and $V_{64}O$, but these workers interpreted their diffraction patterns in terms of a compound $Ta_{32}O_9$.

We wish to point out that the results of these latter investigations (refs. 4,6) can also be completely accounted for by the $Ta_{64}I$ superlattice

(where I represents the interstitial, in these cases probably carbon) and not in terms of $Ta_{32}O_9$. Geiss and Lawless, in fact, point out that they cannot explain all the observed spots on the basis of a $Ta_{32}O_9$ superlattice. Our arguments and interpretations of the results of refs. 4,6 in terms of $Ta_{64}I$ follow exactly those already published in references 1,2 and there seems no need to repeat them again now. Further doubt on the $Ta_{32}O_9$ proposal is provided by the results of van Landuyt and Wayman[5] who also investigated the Ta-O system and identified the sub-oxide TaO_y (orthorhombic).

The data obtained thus far on interstitially ordered Group V B metals containing carbon, nitrogen, oxygen confirm the predictions made by Beshers in that the structures identified by electron diffraction are consistent with the models he proposed for the expected interstitial site occupancies. According to Beshers' calculations,[9] oxygen and nitrogen in tantalum and niobium as well as nitrogen and carbon in vanadium should prefer tetrahedral site occupancy, whereas carbon and nitrogen in α-iron, carbon in tantalum, and oxygen in vanadium should prefer octahedral sites. Therefore, according to these calculations, carbon in tantalum and oxygen in vanadium, occupying octahedral sites, should give rise to similar ordered phases, as is observed (1,2,3).

It must be noted, however, that the $Ta_{64}C$ structure reported by Villagrana and Thomas[1] exists only at the critical {1.56 atomic percent carbon} composition. At all other stages, a state of partial order exists. It has been shown that the final $Ta_{64}C$ structure is obtained by the superposition of four sets of carbon composition fluctuations along the $\{110\}_{Ta}$ planes such that $\lambda_{\{110\}_C} = 4d_{\{110\}_{Ta}}$.[7] The b.c.t. $Ta_{64}C$

structure occurs only when the carbon atom positions are uniquely defined by four simultaneous sets of carbon compositon fluctuations along the {110} planes. The $Ta_{64}C$ structure is, therefore, a "macroscopic" structure, composed of regions wherein the degree of order may vary. The structure is correct, however, in terms of chemical composition (that is, 1.56 atomic percent carbon) as shown by Helium-3 activation analysis. A more detailed account of the development of the superlattice as a result of interstitial ordering will be reported later.[8]

Acknowledgements

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