



Fig. 1. The structure of $Ti_{2+x}S_4$ viewed down the a axis. Sulphur atoms are drawn as larger circles, completely filled Ti_1 sites as small black circles, and partly occupied Ti sites as crosses. The unit cell is drawn in projection with broken lines.

The titanium atoms are each distant 2.45 \AA from six sulphurs at the corners of a nearly regular octahedron, and have an additional metal 2.86 \AA away as a seventh

neighbour through the centre of an octahedral face. In each octahedron there are six S-S distances of 3.43 \AA (the a axis length) and six of 3.48 \AA . The Ti-Ti distance in metallic titanium is 2.90 \AA , and it is possible that some form of metal-to-metal bonding exists between adjacent octahedra sharing a face parallel to (0001). The two sulphur atoms have different environments, S_1 is at the centre of a trigonal prism of titanium atoms, whilst S_2 is at the centre of an octahedron.

Many of the sesqui-selenides and -tellurides of the transition metals may perhaps be regarded as the 'averaged mean' of the closely related $C6$ and $B8$ structures. TiS_2 has the $C6$ arrangement, whilst in the high-temperature form of TiS the $B8$ grouping is modified by regular stacking disorders (Hahn & Harder, 1956). The non-stoichiometric titanium 'sesquisulphide' therefore represents a transitional or intermediate structure between the two.

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Lattice parameters of cold-worked Cu-Zn-Ga alloys. By L. CASTELLIZ, C. S. BARRETT and T. B. MAS-SALSKI,* *Institute for the Study of Metals, University of Chicago, Chicago, Illinois, U.S.A.*

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Massalski & Barrett (1957) have recently shown that ternary Cu-Zn-Ga alloys with the body-centered cubic structure, in the region of the equilibrium diagram where this high-temperature structure can be retained by a rapid quench, can be subsequently transformed by cold working.

Three such alloys, falling along the line of constant valence-electron:atom ratio ($e/a = 1.476$), have been subjected to cold work after quenching from the b.c.c. region, and the lattice parameters of the transformation structure are reported in this note.

The alloys were obtained from materials of 99.98-99.99% purity, cast in 'Vycor' tubing, homogenized at

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Table 1. *Lattice parameters*

Alloy*	Composition (atomic%)			Lattice parameter (Å)
	Cu	Zn	Ga	
1 Ga	54.9	42.5	2.6	3.730 ± 0.002
2 Ga	57.4	37.5	5.1	3.717 ± 0.002
D5	65.07	23.67	11.26	3.705 ± 0.002

* Alloy designations are the same as those used by Massalski & Barrett (1957).

800° C. and quenched in brine. Their composition is given in Table 1. X-ray patterns were obtained with monochromatized $\text{Cu } K\alpha$ radiation in a G. E. X-ray diffraction unit. After filing at room temperature, and immediate X-ray exposure, lines of a transformation structure were

observed in addition to lines of the untransformed b.c.c. phase. The new lines corresponded to a heavily faulted close-packed hexagonal structure in alloys near the Cu-Ga binary axis, gradually changing into a faulted structure showing both the face-centered cubic and close-packed hexagonal characteristics near the Cu-Zn binary axis (Massalski & Barrett, 1957).

In Table 1 are shown lattice parameters of the transformation structure calculated from the 311 reflections of Debye-Scherrer patterns, indexed as f.c.c.

Deformation faulting causes shifts of certain reflections in the f.c.c. Debye-Scherrer pattern (Paterson, 1952)

but it was found that in the case of binary Cu-Zn alloys (Massalski & Barrett, 1957) lattice-parameter values could be estimated with reasonable precision using the assumption that the 311 reflection remained practically unshifted by the presence of faults.

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Atomic scattering factors for Mo⁺.* By EDGAR L. EICHHORN, *The California Institute of Technology, Pasadena, California, U.S.A.*

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For the heavier elements the earliest scattering curves were approximated by James & Brindley (1931) with an interpolation method based upon the Thomas-Fermi treatment in which the atomic electron cloud is considered in terms of a degenerate gas. The scattering curves for molybdenum have not been corrected since; however in 1955 accurate self-consistent wave-field data for the molybdenum monovalent positive ion became available through the work of the Hartree school in Cambridge. The present computation of the new scattering curve (Table 1 and Fig. 1) is based upon the self-consistent

field data, calculated by Ridley (1955) on the Cambridge E.D.S.A.C. computer.

It was decided to undertake the programming of the calculation of scattering curves from wave-field data in general form, so that other elements could be computed also. The digital computer at C.I.T., an ElectroData Datatron, was utilized for this purpose. The numerical integration of expressions of the form

$$\int_0^{\infty} \frac{P_j^2(r) \cdot \sin 4\pi\sigma r}{4\pi\sigma r} \cdot dr$$

(where $P_j(r)$ is the radially dependent part of the wave function for shell j at distance r (in Bohr units) from the nucleus, and $\sigma = \sin \theta/\lambda$) is carried out by a curve-fitting procedure, the accuracy of which is of the same order as

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Table 1. *Atomic scattering factors for Mo⁺*

$\frac{\sin \theta}{\lambda} \times 10^{-8}$		$\frac{\sin \theta}{\lambda} \times 10^{-8}$		$\frac{\sin \theta}{\lambda} \times 10^{-8}$		$\frac{\sin \theta}{\lambda} \times 10^{-8}$	
(cm.)	$f(\text{Mo}^+)$	(cm.)	$f(\text{Mo}^+)$	(cm.)	$f(\text{Mo}^+)$	(cm.)	$f(\text{Mo}^+)$
0.00	41.00	0.46	22.48	0.92	13.78	1.38	8.43
0.02	40.85	0.48	21.96	0.94	13.48	1.40	8.26
0.04	40.44	0.50	21.47	0.96	13.17	1.42	8.13
0.06	39.77	0.52	21.01	0.98	12.89	1.44	7.98
0.08	38.93	0.54	20.56	1.00	12.59	1.46	7.86
0.10	37.95	0.56	20.14	1.02	12.32	1.48	7.73
0.12	36.90	0.58	19.71	1.04	12.04	1.50	7.62
0.14	35.81	0.60	19.32	1.06	11.76	1.52	7.48
0.16	34.71	0.62	18.92	1.08	11.51	1.54	7.38
0.18	33.62	0.64	18.54	1.10	11.25	1.56	7.26
0.20	32.53	0.66	18.16	1.12	11.01	1.58	7.16
0.22	31.51	0.68	17.80	1.14	10.75	1.60	7.06
0.24	30.52	0.70	17.43	1.16	10.53	1.62	6.98
0.26	29.58	0.72	17.07	1.18	10.30	1.64	6.88
0.28	28.68	0.74	16.73	1.20	10.09	1.66	6.80
0.30	27.83	0.76	16.38	1.22	9.87	1.68	6.71
0.32	27.01	0.78	16.04	1.24	9.67	1.70	6.63
0.34	26.25	0.80	15.70	1.26	9.46	1.72	6.55
0.36	25.55	0.82	15.38	1.28	9.28	1.74	6.47
0.38	24.84	0.84	15.04	1.30	9.10	1.76	6.41
0.40	24.21	0.86	14.71	1.32	8.93	1.78	6.33
0.42	23.59	0.88	14.39	1.34	8.75	1.80	6.26
0.44	23.03	0.90	14.09	1.36	8.59		