Acta Cryst. (1963). **16**, 1183

The crystal structure of $MoSe_2$.*

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(*Received* 27 *August* 1962 *and in revised form* 20 *May* 1963)

Crystal structures of the compounds of tetravalent molybdenum and tungsten with elements of Group VIA of the periodic table are being examined as part of a program to determine the effect of crystal structure on friction properties.

Table 1. *X-ray data for* $MoSe_2$

hkl	d_o	d_c	I_o†	I_c ($\mu=\frac{5}{8}$)
002	6·44	6·46	78	86
004	3·225	3·232	6	6
100	2·839	2·848	63	63
101	2·788	2·781	6	20
102	2·617	2·606	7	10
103	2·369	2·376	100	100
006	2·151	2·153	10	4
105*	1·914	1·914	39	46
110*	1·641	1·644	49	25
008	1·615	1·616	13	8
112	1·591	1·593	10	8
114	1·464	1·465	2	1
200	1·422	1·424	8	4
203*	1·352	1·352	13	11
116	1·306	1·307	6	3
205*	1·246	1·247	8	8
118	1·152	1·152	33	11
1,0,11	1·087	1·086	4	4
210	1·076	1·076	3	2
213*	1·044	1·044	14	8
215	0·9930	0·9936	8	8
300	0·9492	0·9492	6	4
1,0,13	0·9389	0·9389	4	3
2,0,11	0·9060	0·9064	4	3
306	0·8685	0·8685	1·5	1·2
220	0·8220	0·8220	5	5
308	0·8185	0·8185	13	10
0,0,16	0·8080	0·8081	2	2
1,1,14	0·8052	0·8052	3	1
2,1,11	0·7939	0·7938	9	14
310	0·7897	0·7897	4	4

* Indicates overlapping Si lines. Intensities are corrected.

† Intensities were measured with a double-beam microdensitometer.

* This work was supported by Directorate of Materials and Processes, Aeronautical Systems Division, United States Air Force.

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Samples used were prepared by K and K Laboratories. From X-ray analysis the $MoSe_2$ sample appeared to be of high purity, but the $MoTe_2$ was found to contain large amounts of free tellurium. Structures were determined from powder diffraction photographs made with filtered Cu $K\alpha$ radiation. Approximately 40% silicon was added to one sample as a check on the calibration of the camera.

The powder pattern resembles that of MoS_2 and the structures are isomorphous. $MoSe_2$ is hexagonal, belonging to space group $P6_3/mmc$ (D^4_{6h}), with 2 $MoSe_2$/unit cell. Atomic coordinates of $MoSe_2$ are the same as those of MoS_2 with Mo at $\pm(\frac{1}{3}, \frac{2}{3}, \frac{1}{4})$ and Se at $\pm(\frac{1}{3}, \frac{2}{3}, \mu)$ and $\pm(\frac{2}{3}, \frac{1}{3}, \mu+\frac{1}{2})$. μ is approximately $\frac{5}{8}$. Intensities calculated for $\mu=\frac{5}{8}$ are compared in Table 1 with the observed intensities. The intensities were computed relative to the 103 reflection; standard corrections were used for polarization, multiplicity, and the Lorentz factor (see *e.g.* Klug & Alexander, 1954).

Lattice parameters of $MoSe_2$ were determined by averaging the parameters calculated from the six lines of largest θ. The parameters at 26 °C were found to be:

$$a = 3.288 \pm 0.001 \text{ Å}, \quad c = 12.931 \pm 0.004 \text{ Å}.$$

The calculated density is 6.96 g.cm^{-3}. Interatomic distances calculated from this structure are:

(6) Mo–Se 2.49 Å
(6) Se–Se 3.29
(1) Se–Se 3.23
(3) Se–Se 3.75

A study of $MoTe_2$ yielded results in agreement with those reported by Puotinen & Newnham (1961).

The authors are grateful for the valuable discussions with Dr. R. Peavler of Midwest Research Institute.

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