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A note on the structure of tungsten carbide.

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The B_h(WC) type of structure was hitherto described in two ways:

either D^1_{6h}, $P6/mmm$, with

1 W: in 1 *a* 0, 0, 0 .

1 C at random in 2 *d* $\frac{1}{3}, \frac{2}{3}, \frac{1}{2}$; $\frac{2}{3}, \frac{1}{3}, \frac{1}{2}$.

or D^1_{3h}, $P\bar{6}m2$, with

1 W: in 1 *a* 0, 0, 0 .

1 C: in 1 *d* $\frac{1}{3}, \frac{2}{3}, \frac{1}{2}$.

or 1 *f* $\frac{2}{3}, \frac{1}{3}, \frac{1}{2}$.

The lattice constants are:

$a = 2{\cdot}9065$, $c = 2{\cdot}8366$ Å (Pearson, 1958) .

These alternatives can be readily distinguished using the neutron-diffraction method since the coherent scattering amplitude of thermal neutrons for carbon is $0{\cdot}66.10^{-12}$ cm. as compared with $0{\cdot}47.10^{-12}$ cm. for tungsten.

The experiment was carried out using 1·41 Å neutrons reflected from an Al monochromator cut along the (100) plane. The proportion of second-order radiation in the monochromatic beam was found to be 5%. Measurements up to $2\theta = 80°$ were made automatically on the neutron spectrometer designed by Blinowski (1958).

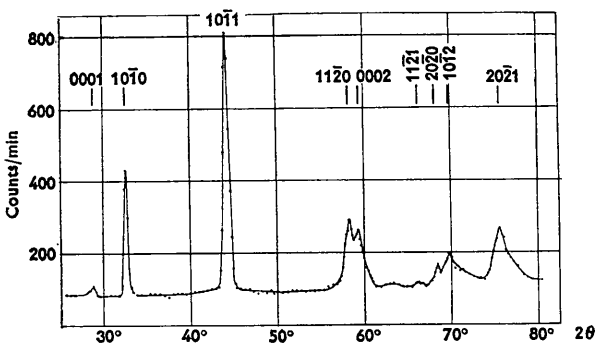

Fig. 1. Neutron diffraction pattern of WC.

Counts were taken each 10′ of scattering angle in the peak area and each 30′ on the background line. The counting time was 14 min. WC powder, 2μ grain size, analytically and X-ray controlled, contained in an aluminium tube 15 mm. in diameter was used. A neutron-diffraction pattern of WC is shown on Fig. 1. A summary of observed and calculated intensities is given in Table 1.

Table 1. *Neutron diffraction data for* WC

hkil	I_o	I_c for space group $P6/mmm$	I_c for space group $P\bar{6}m2$
0001	1	0·67	0·67
10$\bar{1}$0	13	0·79	13·10
10$\bar{1}$1	43	28·90	42·70
11$\bar{2}$0	16	18·40	18·40
0002	8	5·88	5·88
11$\bar{2}$1	1	0·95	0·95
20$\bar{2}$0	4	0·23	3·57
10$\bar{1}$2	8	0·45	7·36
20$\bar{2}$1	18	13·60	19·25

The R factor defined as:

$$R = \Sigma(I_o - I_c)/\Sigma I_o$$

is 0·47 for $P6/mmm$ and 0·07 for $P\bar{6}m2$. This leaves no doubt that the space group for B_h type of structure should be $P\bar{6}m2$ with:

1 W: in 1 *a* 0, 0, 0 .

1 C: in 1 *f* $\frac{2}{3}, \frac{1}{3}, \frac{1}{2}$.

For this case the temperature factor as determined from the slope of the plot of logarithm of I_o/I_c versus $\sin^2\theta/\lambda^2$ is $2B = 2{\cdot}22$ Å^2.

References

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On the setting of crystals for X-ray diffraction work.

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While attempting to orientate a cleavage fragment of a highly absorbing mineral in an X-ray diffraction camera, we were faced with a small difficulty which led to an improvement in the technique used for setting a given zone axis parallel to the rotation axis of the camera.

The technique usually employed when the zero layer line is recognizable on the film and the misorientation is small is that of Weisz & Cole (1948) which makes use of a double oscillation (or a double Laue) photograph in combination with the formulae of Hendershot (1937):

$$\begin{aligned} d_\perp &= R \sin 2\theta \sin i_\perp \\ d_{||} &= R(1 - \cos 2\theta) \sin i_{||} , \end{aligned} \qquad (1)$$

where R is the radius of the cylindrical camera; $i_\perp$ and $i_{||}$ are the angular errors on the two arcs of the goniometer