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The structure of a silicon carbide polytype 24*R*.

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During the course of investigations on growth phenomena in silicon carbide (Knippenberg, 1963) a crystal specimen consisting of two intergrown platelets was found in a batch of crystals prepared by a modified Lely procedure. X-ray diagrams showed weak continuous streaks due to stacking disorder and sharp reflexion spots corresponding to the known polytypes 6*H*, 21*R* and 8*H* and to a new 24-layer structure having rhombohedral symmetry: 24*R*.

It turned out to be possible to isolate this last modification by sawing and grinding. In the final sample, a small rectangular bar with dimensions $1{\cdot}1 \times 0{\cdot}2 \times 0{\cdot}1$ mm, the absence of all other structures and of the stacking disorder was verified by means of strongly overexposed X-ray photographs.

The Laue symmetry of the crystal is $R\bar{3}2/m$, so that the space group must be $R3m$ if this structure — like all SiC structures known to date — is close-packed, each atom being surrounded tetrahedrally by four atoms of the other kind. Eventually, this seemingly trivial assumption is confirmed by the agreement between observed and calculated intensities.

From Weissenberg photographs calibrated with aluminum powder lines the edges of the hexagonal unit cell were determined: $a = 3{\cdot}082 \pm 0{\cdot}003$ and $c = 60{\cdot}49 \pm 0{\cdot}01$ Å. The wavelengths of copper $K\alpha_1$, $K\alpha_2$ and $K\beta$ radiation and the unit-cell edge of aluminum were taken from *International Tables for X-ray Crystallography* (1962).

In order to ascertain the structure of an n-layer polytype it is sufficient to compare the observed and calculated intensities of the reflexions $10l$ with l ranging from $+n$ to $-n$ (Krishna & Verma, 1964). For this purpose the crystal was oriented along the direction of its longest edge, which coincides with the hexagonal a axis, and a set of zero-level, Mo $K\alpha$, Weissenberg photographs of different exposure times was made. The relative intensities of 16 reflexions $10l$ ($+24 > l > -24$) were estimated visually by means of a calibrated film strip. In reducing observed intensities to $|F_o|^2$ values the absorption corrections were neglected ($\mu d < 0{\cdot}5$).

It can be shown that there are eight possible SiC–24*R* structures. These structures have the following Zhdanov symbols: $(35)_3$, $(62)_3$, $(5111)_3$, $(1124)_3$, $(4121)_3$, $(1223)_3$, $(121211)_3$ and $(131111)_3$. The corresponding $|F_c|^2$ values are listed in Table 1 together with the observed intensity data. Evidently, the present structure must be represented by $(35)_3$.

The atomic coordinates are:

8 Si at 000, 00.3z, 00.6z, 00.10z, 00.12z, 00.15z, 00.17z, 00.21z,

8 Si at $\frac{2}{3}$, $\frac{1}{3}$, $\frac{1}{3}$ plus the above coordinates,

8 Si at $\frac{1}{3}$, $\frac{2}{3}$, $\frac{2}{3}$ plus the above coordinates,

where $z = \frac{1}{24}$, and

24C, one above each Si, at a distance $p = \frac{1}{8}\frac{1}{2}$ having coordinates 00p plus the coordinates of the 24 Si atoms.

The *ABC* sequence is

ABCACBACBCABACBACABCBACB .

All α-SiC structures so far determined have been described by Zhdanov symbols containing the numbers 1, 2, 3, 4 and 6. The structure reported here presents the first example of a 5-sequence.

A paper on the optical properties of this polytype will appear soon (Zanmarchi, 1964).

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Table 1. *Observed and calculated values of* $|F(10l)|^2$

		$\|F_c\|^2 \times 10^{-2}$							
l	$\|F_o\|^2$	$(35)_3$	$(62)_3$	$(5111)_3$	$(1124)_3$	$(4121)_3$	$(1223)_3$	$(121211)_3$	$(131111)_3$
22	6	7	13	20	7	2	25	93	50
19	23	22	13	1	32	15	39	6	13
16	81	90	14	4	47	4	25	4	14
13	60	58	34	37	119	15	162	216	187
10	88	94	188	282	94	351	25	7	50
7	95	98	333	152	14	39	73	26	6
4	58	51	0	51	51	153	51	51	0
1	6	4	13	85	80	57	26	15	125
$\bar{2}$	23	15	30	45	15	4	56	209	112
$\bar{5}$	72	70	41	3	102	47	125	19	43
$\bar{8}$	242	285	46	11	148	11	80	11	46
$\bar{11}$	84	83	49	53	171	21	232	310	269
$\bar{14}$	53	47	94	141	47	175	13	3	25
$\bar{17}$	33	28	96	44	4	11	21	8	2
$\bar{20}$	22	17	0	17	17	52	17	17	0
$\bar{23}$	2	2	7	43	40	29	13	7	64
$R^*=$		11%	96%	102%	60%	120%	81%	135%	126%

* $R = \Sigma\,||F_o|^2 - |F_c|^2| / \Sigma |F_o|^2$.