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Some remarks on the Ott's interval sequence in SiC polytypes.*

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The restriction of Ott's interval sequence in the polytypes of SiC to the numbers 2, 3 and 4 is related to the fact that 1 does not normally occur in the Zhdanov symbol.

There seems to be no explanation available in the literature of the fact that Ott's interval sequence (Ott, 1925) in the polytypes of SiC is restricted to the numbers 2,3, and 4 only. (See Verma & Krishna, 1966.) The purpose of this note is to point out that this observation finds a ready explanation if taken in conjunction with the other observed feature of SiC polytypes, namely, that the number 1 does not normally occur in the Zhdanov symbol. [The polytype 2*H* with symbol 11 is an exception. For a recent review see Shaffer (1969).] Since the interval sequence pertains to the three symmetry axes A, B, C (Fig. 1) of the hexagonal lattice, discussion becomes simplest if we consider the $(11\bar{2}0)$ plane depicting Ramsdell's zigzag sequence (Ramsdell, 1947). Consider first a polytype based on a hexagonal lattice. Any sequence of numbers such as $n_1, n_2, n_3 \ldots$ in the Zhdanov notation is equivalent to making successively n_1 steps to the right (say), then n_2 to the left and n_3 to the right and so on, these steps being always along the diagonal as indicated in Fig. 1.

(I) Consider first the case when $n_1, n_2, n_3 \ldots$ are all greater than or equal to 3. In this case it is obvious, because of the fact that any three consecutive steps in the same direction take one to a point equivalent by translational symmetry, that the problem is reduced to one of considering n_j modulo 3. Thus it reduces to considering sequences where the n_j involve 3, 2 or 1.

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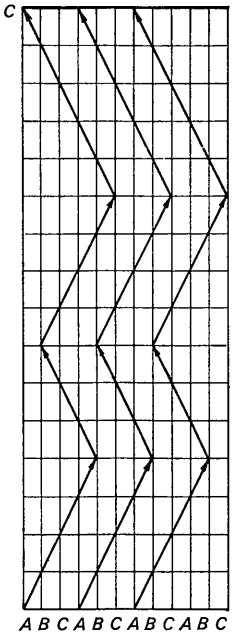

Fig. 1. A hypothetical polytype 21*H* with Zhdanov symbol 4345.

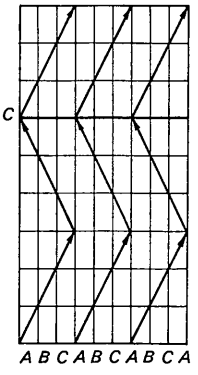

Fig. 2. Polytype 6*H*, with Zhdanov symbol 33.

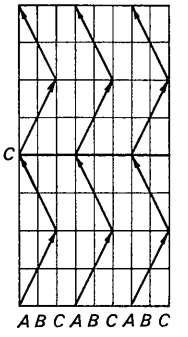

Fig. 3. Polytype 4*H*, with Zhdanov symbol 22.

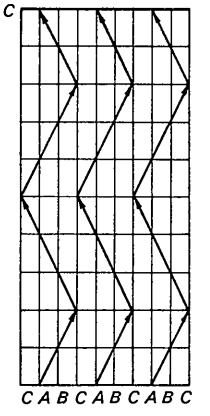

Fig. 4. Polytype 10*H*, with Zhdanov symbol 2332.

(II) Consider the case when all n_j are equal to 3. It is readily seen from Fig. 2 that the interval becomes 3 for axis *A*, and 2 and 4 for axes *B* and *C*.

(III) If we take the case when all are equal to 2 and starting from *A* (say), it is seen that the interval becomes 4 for axes *A* and *C* while it is 2 for axis *B*. (Fig. 3).

(IV) If in the sequence $n_1, n_2, n_3 \ldots$ 2's are sandwiched between 3's, then again the results of cases (II) and (III) become operative and thus any combination of 3's and 2's produces only intervals of 2, 3 and 4 and none greater than 4 (Fig. 4).

The case in which the interval can be greater than 4 can be realized only if 1's are involved in the Zhdanov symbol. Thus a sequence of complete 1's (polytype 2*H*) produces intervals of 2 in two of the axes while the third axis is completely unoccupied (it may be considered to be of infinite interval). This infinite interval can be brought down to a finite one of any desired value if an appropriate sequence of 1's is sandwiched by n_1 and n_2, with both n_1 and $n_2 \geq 2$. (Fig. 5). Thus, the interval sequence need not be restricted to 2, 3 and 4 provided 1's occur in the Zhdanov symbol. This is not the case in SiC polytypes, and the observed intervals of 2, 3 and 4 can thus be attributed to the absence of 1's in the Zhdanov symbol. These remarks can be readily extended to the rhombohedral lattice where the axes *A*, *B* and *C* become equivalent.

The non-occurrence of 1's in the Zhdanov symbol might itself find an explanation from a physical mechanism, such as for instance Mitchell's (1957) treatment based on screw dislocations, and the generation of certain family series of polytypes or from Schneer's (1955) treatment. These, however, need not concern us here.

I should like to thank Dr A. R. Verma for helpful comments.

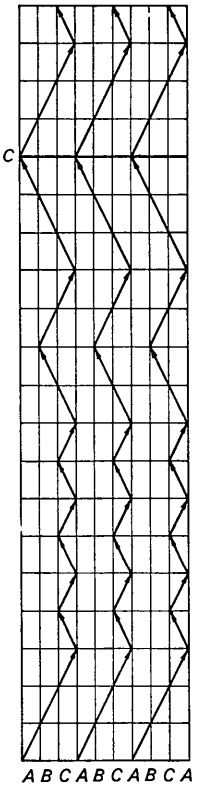

Fig. 5. Hypothetical polytype 16*H* with Zhdanov symbol $3(11)_3223$. Note an interval of 10 occurring along *B*.

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A clarification of differences in site orientation in crystals.

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Tables are presented whereby physically relevant differences in the relationship of the elements of symmetry of a Wyckoff site to those of the crystal class can be distinguished.

In *International Tables for X-ray Crystallography*, (1969) the various sets of equivalent points (Wyckoff sites) are described by the point group of the elements of symmetry passing through a typical point (*i.e.* the site group), the number of points in the set, their coordinates, the Wyckoff label and some information of relevance to X-ray crystallographers. For those interested in spectroscopic and other tensorial properties of crystals, however, this is often insufficient and a detailed examination of the coordinates has hitherto been necessary in some cases where differences in site orientation within the unit cell can lead to different correlations of the representations of the crystal class and those of the site group.

The problem can be illustrated simply by means of the crystal class $D_2 = 222$. A site of symmetry $C_2 = 2$ can lie on the crystallographic *x*, *y* or *z* axes of the unit cell and accordingly the correlation between the representations of D_2 and C_2 is given on descent in symmetry by the subgroup table

D_2	C_2^x	C_2^y	C_2^z
A	*A*	*A*	*A*
B_1	*B*	*B*	*A*
B_2	*B*	*A*	*B*
B_3	*A*	*B*	*B*

and on ascent in symmetry by the supergroup tables