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A simplified method of generating layer sequences for SiC polytypes

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According to the principle that high-temperature phases of SiC should not have "1" in the Zhdanov notation of their layer sequences, a simplified method of generating the layer sequences has been designed. This method is described in order that all of the possible layer sequences without "1" may be generated systematically. By utilizing this method, full sets of the possible layer sequences of SiC polytypes up to 20-layers are produced.

1. Introduction

About 160 different polytypes of SiC crystals have so far been reported, and structures have been assigned to about one-half of these [1–4]. SiC is one of the typical substances which exhibit a phenomenon of polytypism and it is expected that more new polytypes will be discovered in the future.

For structure analysis of SiC polytypes, the trial-and-error method is usually employed. The generation of all of the possible layer sequences which is necessarily involved in this method, however, becomes quite troublesome with increased layer numbers. In order to avoid this difficulty, the author has introduced the principle of exclusion of "1" from the Zhdanov notation and thus succeeded in the structure determination of such SiC polytypes as 45R [5], 21T [6], 20H(a) and 20H(b) [7]. Since it is believed that this principle is an indispensable guide for the determination of SiC structures, a description of a simplified method for deriving systematically the full sets of possible layer sequences will be attempted in this paper.

2. Significance of "1" in the Zhdanov notation

2.1. Zhdanov numbers of SiC

Each integer of a Zhdanov notation used for the representation of polytype structures will be specified as a "Zhdanov number" in the following discussion. Thus, each Zhdanov number is the number of layers in the structure which are stacked together in sequence in only one direction without comprising a "fold" and a polytype structure can be represented by the series of Zhdanov numbers.

As the natural limitation imposed upon the layer sequences in SiC polytypes, Zhdanov and Minervina [8] assumed that the Zhdanov numbers of every actually realized structure should consist of only 2s and 3s, and successfully derived the layer sequence of 51R as $((33)_2 32)_3$. Ramsdell [9] determined the structure of 33R, $(3332)_3$ under the assumption that no number other than 2, 3 and 4 should appear. Krishna and Verma [10], with the same assumption, succeeded in the analysis of 57R, $(333334)_3$. However, further new polytypes such as 174R$((33)_3 6(33)_5 4)_3$ by Tomita [11], 24R$(53)_3$ by Knippenberg [12] and Gomes de Mosquita [13], 9T(63) by Inoue *et al.* [14], 81H$((33)_5 35(33)_6 34)$ by Nishida [15] have since been discovered, thus allowing such numbers as 5 and 6 to appear in addition to 2, 3 and 4. Therefore, some new polytypes having larger numbers than 6 might well be discovered in the future.

2.2. Zhdanov number "1"

Since the polytype 2H was discovered by Adamsky and Merz [16], this polytype has been treated uniquely from the other types owing to its peculiarity of having the Zhdanov number "1", because "1" has never been found in the structures of any other polytypes belonging to the high-temperature phase. Moreover, according to the thermodynamic investigations, it has been con-

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firmed that 2H is a low-temperature phase formed below 1400° C [17, 18], and that it is transformed into 3C, 4H and 6H with a rise in temperature, changing to 3C at 1600° C, to 4H at 1900° C and to 6H to 2000° C [19, 20].

Therefore, from these expermental results, the author maintains that every SiC polytype of a high-temperature phase, i.e. a polytype grown over 2000° C should not have "1" in the Zhdanov number of its layer sequence. In fact, it will be found in Part 2 that this principle plays an important part in the structure analysis of other complicated polytypes [5–7].

2.3. Exclusion of "1"

At the present state of the art of X-ray crystallography, the trial-and-error method is the universally adapted precedure for analysis of SiC structures. The difficulty will rapidly increase as the c-period of the crystal becomes longer, however, and even for structures with a layer less than 20, the process of generating the possible layer sequence easily exceeds the capacity of a modern high-speed computer. On the other hand, if the principle of exclusion of "1" from the Zhdanov number is adopted, the state of affairs will be greatly remedied and the process of generating necessary layer sequences will be brought back into a magnitude manageable with an ordinary computer, the only exception being when the layer number is prohibitively large. As an example, all of the possible layer sequence up to the 12-layered periodicity [21] are given in Table I. If we now exclude from the table those bearing "1" in the Zhdanov notation, we have Table II and realize how large an amount of labour can be saved in the structure determination, provided that the principle of exclusion of "1" holds.

3. Generation of full sets of the possible layer sequences for SiC polytypes

In order to generate all of the possible layer sequences of SiC polytypes, the author has proposed a way of using a computer to find all of the

TABLE I All possible layer sequences up to 12 layers

N	Theoretically possible layer sequences: Hexagonal, trigonal	Rhombohedral
2	11	–
3	–	21
4	22	31
5	41	32, 2111
6	33, 2112	42, 513111
7	52, 4111, 3121	61, 43, 2212, 211111, 3211
8	71, 44, 121121, 3113, 211112, 3212	62, 41, 21, 5111, 53, 311111, 211121, 4211, 3221
9	63, 3132, 411111, 5211, 4221, 312111	4311, 3321, 3222, 311211, 72, 54, 321111, 221211, 222111, 81, 6111, 5121, 21111111, 4131, 4212
10	82, 7111, 6121, 5131, 4312, 321211, 321112, 55, 131131, 212212, 4114, 3223, 311113, 221122, 21111112, 12111121	64, 4222, 411211, 221212, 91, 73, 511111, 312121, 311131, 5212, 3313, 31111111, 21111121, 6211, 5221, 4231, 412111, 5311, 4321, 421111, 322111, 321121, 312211
11	10.1, 74, 6212, 5222, 4232, 511211, 312221, 311132, 41111111, 31112111, 6311, 21211121, 5321, 4331, 521111, 422111, 421121, 412211, 313211, 322121, 31211111	92, 8111, 7121, 6131, 5141, 83, 4142, 611111, 412121, 213131, 7211, 6221, 5231, 512111, 413111 26 cases omitted
12	93, 711111, 512121, 414111, 8211, 7221, 6231 5241, 612111, 513111, 413121, 66, 411411, 2111121111, 5115, 4224, 411114, 321123, 231132, 312213, 22111122, 21211212, 31111113, 5313, 13111131, 2111111112, 1211111121, 4323, 421212, 22112112, 22111221, 32111112, 5412, 342111, 312411, 312114, 332211, 322212, 32121111, 32111211, 123123, 31121211	11.1, 10.2, 9111, 8121, 7131, 6141 64 cases omitted

TABLE II Possible layer sequences derived from Table I by excluding the Zhdanov number "1"

Number of layers	Stacking sequences	
	Hexagonal, trigonal	Rhombohedral
2	–	–
3	–	–
4	22	–
5	–	32
6	33	42
7	52	43
8	44	62, 53
9	63	72, 54, 3222
10	82, 55, 3322	73, 64, 4222
11	74, 5222, 4232	92, 83, 65, 4322, 3332
12	93, 66, 4422, 4323	10.2, 84, 75, 6222, 5322, 5232, 4332

sequences in the integers which are produced from even combinations of Zhdanov numbers. This method will be systematically described in the following four sections.

3.1. Combination of Zhdanov numbers

Initially, a complete set of all combinations of Zhdanov numbers must be determined. If we represent the "complete set" as C_N for a given layer number N, the complete sets up to 10 layers will be given as follows:

$$C_2 = \{2\}$$
$$C_3 = \{3\}$$
$$C_4 = \{4, 22\}$$
$$C_5 = \{5, 32\}$$
$$C_6 = \{6, 42, 33, 222\}$$
$$C_7 = \{7, 52, 43, 322\}$$
$$C_8 = \{8, 62, 53, 44, 422, 332, 2222\}$$
$$C_9 = \{9, 72, 63, 54, 522, 432, 333, 3222\}$$
$$C_{10} = \{10, 82, 73, 64, 622, 55, 532, 442, 433, 4222, 3322, 22222\}$$

An integer p may now be adjoined to a complete set C_N, so as to form another set of combinations which will be called the "adjoined set" and be represented as $p \cdot C_N$. For example, if integer 9 is adjoined to the complete set C_6, the adjoined set of combination is determined to be

$$9 \cdot C_6 = \{96, 942, 933, 9222\}.$$

Next, we will define the derived set $p \cdot C'_N$. A subset of an adjoined set $p \cdot C_N$ is called a "derived set" if each combination of Zhdanov numbers in C_N consists of integers not greater than p. Therefore, if $p \geqq N$, the derived set $p \cdot C'_N$ coincides with the adjoined set $p \cdot C_N$, but if $p < N$, the derived set is a proper subset of the adjoined set. For example, for $N = 10$ and $p = 5$,

$$5 \cdot C'_{10} = \{555, 5532, 5442, 5433, 54222, 53322, 522222\}.$$

Then, C_N can be given, if N is even ($m = N/2$), as

$$C_N = N + \sum_{j=2}^{m} (N-j) \cdot C_j + \sum_{j=1}^{m-2} (m-j) \cdot C'_{m+j}$$

and, if N is odd ($m = (N-1)/2$), as

$$C_N = N + \sum_{j=2}^{m} (N-j) \cdot C_j + \sum_{j=1}^{m-2} (m-j+1) \cdot C'_{m+j}.$$

As an example, let us consider the case of deriving C_{12}:

$$C_{12} = 12 + \sum_{j=2}^{6} (12-j) \cdot C_j + \sum_{j=1}^{4} (6-j) \cdot C'_{6+j}$$

where

$$\sum_{j=2}^{6} (12-j) \cdot C_j = 10 \cdot C_2 + 9 \cdot C_3 + 8 \cdot C_4 + 7 \cdot C_5 + 6 \cdot C_6$$

$$\sum_{j=1}^{4} (6-j) \cdot C'_{6+j} = 5 \cdot C'_7 + 4 \cdot C'_8 + 3 \cdot C'_9 + 2 \cdot C'_{10}.$$

Finally we obtain

$$C_{12} = \{12, 10 \cdot 2, 93, 84, 822, 75, 732, 66, 642, 633, 6222, 552, 543, 5322, 444, 4422, 4332, 42222, 3333, 33222, 222222\}.$$

Consequently, C_{N+1} can be easily derived by using the complete sets of combinations ranging from C_1 to C_N.

3.2. Elimination of odd combinations

Suppose a combination consists of r different integers of Zhdanov numbers, namely, E^1, E^2, E^3, ... , E^r and consists of individually n_1, n_2, n_3, ... , n_r pieces of different integers. Then, the combination can be represented as

$$E_1^1 E_2^1 \ldots E_{n_1}^1 E_1^2 E_2^2 \ldots E_{n_2}^2 \ldots$$
$$\ldots E_1^r E_2^r \ldots E_{n_r}^r,$$

the layer number as

$$N = n_1 \cdot E^1 + n_2 \cdot E^2 + \ldots + n_r \cdot E^r,$$

and the total number of Zhdanov numbers, S, as

$$S = n_1 + n_2 + \ldots + n_r.$$

The combination is called "even combinations" or "odd combination" as S is even or odd, respectively. Then, it is always possible to convert an odd combination into an even combination by adding the Zhdanov numbers at both ends of the odd combination. For instance, an odd combinantion of 64233 should be converted to an even combination of 9423 by adding 6 to 3 at both ends of 64233. The layer structure described by the odd combination is completely equal to that described by the even combination converted from the odd combination. Therefore, only even combinations derived by this method should be taken into consideration and they are listed up to $N = 20$ in Table III.

3.3. Generation of a set of the possible layer sequence from an even combination

Let us consider a set of possible layer sequences which is generated from an initial even combination of Zhdanov numbers. The principle of generation of a set of the possible layer sequence can be described in the following three procedures. These processes were carried out by computer calculation [22].

First, let us obtain the maximum and the minimum integers from an even combination of Zhdanov numbers. When we regard an even combination, $E_1^1 E_2^1 \ldots E_{n_1}^1 E_1^2 E_2^2 \ldots E_{n_2}^2 \ldots E_1^r E_2^r \ldots E_{n_r}^r$, as an integer of S figures, the maximum integer $I_{\max}$ and the minimum integer $I_{\min}$ can be given as

$$I_{\max} = \sum_{j=1}^{n_1} E_j^1 \times 10^{s-j} + \sum_{j=1}^{n_2} E_j^2 \times 10^{s-n_1-j} + \ldots + \sum_{j=1}^{n_r} E_j^r \times 10^{s-(j+n_1+n_2+\ldots+n_{r-1})}$$

$$I_{\min} = \sum_{j=1}^{n_r} E_j^r \times 10^{s-j} + \sum_{j=1}^{n_{r-1}} E_j^{r-1} \times 10^{s-j-n_r} + \ldots + \sum_{j=1}^{n_1} E_j^1 \times 10^{s-(j+n_2+n_3+\ldots+n_r)},$$

where $E^1 > E^2 > \ldots > E^r$ and $S = n_1 + n_2 + \ldots + n_r$.

Secondly, produce every integer ranging from $I_{\min}$ to $I_{\max}$ by adding one by one to $I_{\min}$, and then select all of the integers which do not include the Zhdanov numbers of 0 and 1. All of the possible layer sequences to be produced from an intial even combination should be included among these selected integers provided that each integer is regarded as a Zhdanov number representing a layer sequence. For instance, an even combination of 433222 produces six different layer sequences of 43222, 432232, 423322, 423232, 432322 and 432223 as explained later. In this case, the minimum and maximum integers of six figures are 433222 and 222334, respectively. All of six layer sequences mentioned above are included among the integers of six figures ranging from 222334 to 433222 if each integer is regarded as a Zhdanov number of layer sequences.

Thirdly, regard each of the produced integers as a Zhdanov number of layer sequence, and then choose only Zhdanov numbers whose layer number is equal to that of initial even combination. Consequently, we can obtain a set of the possible layer sequences of identical layer number N without 1 or 0 in the Zhdanov number from an even combination. Each of the even combinations in Table III also produces individually a complete set of possible layer sequences in the same way mentioned here.

Lastly, the full sets of the possible layer sequences are obtained by gathering up each set of possible layer sequences bearing the equal layer number.

TABLE III All even combinations up to 20 layers

N	Combination of Zhdanov numbers
1	–
2	–
3	–
4	22
5	32
6	33, 42
7	52, 43
8	62, 53, 44, 2222
9	72, 63, 54, 3222
10	82, 73, 64, 55, 4222, 3322
11	92, 83, 74, 65, 5222, 4322, 3332
12	10.2, 93, 84, 75, 66, 6222, 5322, 4422, 4332, 3333, 222222
13	11.2, 10.3, 94, 85, 76, 7222, 6322, 5422, 5332, 4432, 4333, 322222
14	12.2, 11.3, 10.4, 95, 86, 8222, 77, 7322, 6422, 6332, 5522, 5432, 5333, 4442, 4433, 422222, 332222
15	13.2, 12.3, 11.4, 10.5, 96, 9222, 87, 8322, 7422, 7332, 6522, 6432, 6333, 5532, 5442, 5433, 522222, 4443, 432222, 333222
16	14.2, 13.3, 12.4, 11.5, 10.6, 10.222, 97, 9322, 88, 8422, 8332, 7522, 7432, 7333, 6622, 6532, 6442, 622222, 5542, 5533, 5443, 532222, 4444, 442222, 433222, 333322, 22222222
17	15.2, 14.3, 13.4, 12.5, 11.6, 11.222, 10.7, 10.322, 98, 9422, 9332, 8522, 8432, 8333, 7622, 7532, 7442, 7433, 722222, 6632, 6542, 6533, 6443, 632222, 5552, 5543, 5444, 542222, 533222, 443222, 433322, 333332, 32222222
18	16.2, 15.3, 14.4, 13.5, 12.6, 12.222, 11.7, 11.322, 10.8, 10.422, 10.332, 99, 9522, 9432, 9333, 8622, 8532, 8442, 8433, 822222, 7722, 7632, 7542, 7533, 7443, 732222, 6642, 6633, 6552, 6543, 6444, 642222, 633222, 5553, 5544, 552222, 543222, 533322, 444222, 443322, 433332, 42222222, 333333, 33222222
19	17.2, 16.3, 15.4, 14.5, 13.6, 13.222, 12.7, 12.322, 11.8, 11.422, 11.332, 10.9, 10.522, 10.432, 10.333, 9622, 9532, 9442, 9433, 922222, 8722, 8632, 8542, 8533, 8443, 832222, 7732, 7642, 7633, 7552, 7543, 7444, 742222, 733222, 6652, 6643, 6553, 6544, 652222, 643222, 633322, 5554, 553222, 544222, 543322, 533332, 52222222, 444322, 443332, 433333, 43222222, 33322222
20	18.2, 17.3, 16.4, 15.5, 14.6, 14.222, 13.7, 13.322, 12.8, 12.422, 12.332, 11.9, 11.522, 11.432, 11.333, 10.10, 10.622, 10.532, 10.442, 10.433, 10.22222, 9722, 9632, 9542, 9533, 9443, 932222, 8822, 8732, 8642, 8633, 8552, 8543, 8444, 842222, 833222, 7742, 7733, 7652, 7643, 7553, 7544, 752222, 743222, 733322, 6662, 6653, 6644, 662222, 6554, 653222, 644222, 643322, 633332, 62222222, 5555, 554222, 553322, 544322, 543332, 533333, 532222, 444422, 444332, 443333, 44222222, 4332222, 33332222, 2222222222

3.4. Circular permutation of Zhdanov number

Identical sequences may exist among the layer sequences produced by the permutation of Zhdanov numbers. For instance, the layer sequences such as 433222, 332224, 322243, 222433, 224332 and 243322 are generated by the permutation of 433222 and they are identical layer sequences each to each. Therefore, it is necessary to take into account circular permutation of Zhdanov numbers in order to avoid the repetition in permutation.

A computer process was carried out to eliminate these identical layer sequences caused by permutation and then all of the possible layer sequences without repetition in permutation can be produced for each even combination. In the case of even combinations of 433222, six different layer sequences of 433222, 432232, 423322, 423232, 432322 and 432223 were produced after the elimination of repetition by the computer procedure.

3.5. Correction for other repetition effects

Some sequences derived by the procedures described above may be found to be composed of a subsequence of shorter period such as 33223322 or 32323232, both derived from the combination of 33332222. In fact, the former is equivalent to the 10-layer sequence of 3322 and the later to be the 5-layer sequence of 32, while 33332222 is a 20-layer sequence. Therefore, care should be taken to eliminate such fictitious sequences appearing during the course of deriving a set of layer sequences. After elimination of such fictitious sequences, the true possible layer sequences can finally be obtained. Full sets of possible layer sequences for SiC polytypes up to 20-layers obtained in this way are tabulated in Table IV.

Further possible layer sequences higher than 20-layers can also be derived successively by the same procedure mentioned above.

4. Conclusions

On the basis of the principle that Zhdanov number "1" should not apear in SiC polytypes grown over 2000° C, all of the possible layer sequences of SiC up to 20 layers, have been generated. If one takes account of the layer sequences bearing "1" in the Zhdanov number, there are, for instance, theoretically 406 possible layer sequences for 15-layered rhombohedral polytypes and 4625 different layer sequences for 20-layered hexagonal and trigonal polytypes [23]. It is indeed remarkable how rapidly the number of possible layer sequences increases as the layer number increases. The simplified method excluding "1" from the Zhdanov number, however, gives us only 22 possible layer sequences for 15-layered rhomgohedral polytypes and only 84 possible layer sequences for 20-layered hexagonal and trigonal polytypes to be taken into consideration as shown in Table IV. It is surprising to find to what extent the principle of exclusion of "1" is capable of reducing the difficulty of structure determination which is

TABLE IV Full sets of possible layer sequences of SiC polytypes up to 20-layers

N	Hexagonal, trigonal	Rhombohedral
1	–	–
2	–	–
3	–	–
4	22	–
5	–	32
6	33	42
7	52	43
8	44	62, 53
9	63	72, 54, 3222
10	82, 55, 3322	73, 64, 4222
11	74, 5222, 4232	92, 83, 65, 4322, 3332
12	93, 66, 4422, 4323	10.2, 84, 75, 6222, 5322, 5232, 4332
13	11.2, 85, 6322, 5332, 4342	10.3, 94, 76, 7222, 6232, 5422, 5242, 5323, 4432, 4333, 322222
14	10.4, 8222, 77, 7232, 6242, 5522, 5423, 4433, 332222, 322322	12.2, 11.3, 95, 86, 7322, 6422, 6332, 6323, 5432, 5342, 5333, 4442, 422222, 323222
15	12.3, 96, 7422, 7323, 6432, 6333, 5442, 5343, 522222, 423222	13.2, 11.4, 10.5, 9222, 87, 8322, 8232, 7242, 7332, 6522, 6252, 6423, 6342, 5532, 5352, 5424, 5433, 4443, 432222, 422322, 333222, 223323
16	14.2, 11.5, 9322, 88, 8332, 7342, 6622, 6523, 6352, 6424, 5533, 5434, 442222, 422422, 432322, 432223, 333322, 332332	13.3, 12.4, 10.6, 10.222, 97, 9232, 8422, 8242, 8323, 7522, 7252, 7432, 7423, 7333, 6532, 6442, 6433, 6343, 622222, 5542, 5452, 5443, 532222, 523222, 522322, 424222, 433222, 432232, 423322, 423232, 333232

TABLE IV (*Continued*)

N	Hexagonal, trigonal	Rhombohedral
17	13.4, 11.222, 10.7, 10.232, 9242, 8522, 8252, 8423, 7262, 8532, 7433, 6542, 6443, 632222, 622322, 5552, 5453, 533222, 532232, 523322, 424223, 422243, 423233, 423332	15.2, 14.3, 12.5, 11.6, 10.322, 98, 9422, 9332, 9323, 8432, 8342, 8333, 7622, 7523, 7352, 7442, 7424, 7343, 722222, 6632, 6362, 6524, 6452, 6533, 6353, 6434, 623222, 5543, 5444, 542222, 524222, 522422, 532322, 532223, 523232, 443222, 422423, 442232, 424232, 433322, 423323, 432233, 432323, 333332, 32222222
18	15.3, 12.6, 10.442, 10.323, 99, 9432, 9333, 8442, 8343, 822222, 7722, 7623, 7524, 7452, 7353, 723222, 6462, 6633, 6534, 624222, 623232, 5544, 552222, 525222, 522522, 532422, 532224, 542322, 523242, 532323, 443322, 443223, 442332, 433422, 432432, 433323, 33222222, 32232222	16.2, 14.4, 13.5, 12.222, 11.7, 11.322, 11.232, 10.8, 10.242, 10.332, 9522, 9252, 9423, 9342, 8622, 8262, 8532, 8523, 8352, 8424, 8433, 7632, 7362, 7542, 7533, 7443, 7434, 732222, 722322, 6642, 6552, 6525, 6543, 6453, 6444, 642222, 622422, 633222, 632322, 632232, 632223, 623322, 5553, 543222, 534222, 532242, 542232, 523422, 524322, 533322, 523233, 523323, 523332, 532233, 444222, 442422, 443232, 434322, 434232, 433242, 432423, 432342, 433332, 433233, 42222222, 32322222
19	17.2, 14.5, 12.322, 11.8, 11.332, 10.342, 9622, 9523, 9352, 9424, 8632, 8362, 8533, 8434, 7372, 7642, 7543, 7444, 742222, 722422, 732322, 732223, 6652, 6553, 6454, 643222, 642232, 623422, 633322, 623323, 632233, 544333, 542242, 524422, 543232, 534322, 534223, 532342, 523432, 533332, 533233, 52222222, 442423, 434332, 444232, 433342, 42322222, 42223222, 32323222	16.3, 15.4, 13.6, 13.222, 12.7, 12.232, 11.422, 11.242, 11.323, 10.9, 10.522, 10.252, 10.423, 10.333, 9262, 9532, 9442, 9433, 9343, 922222, 8722, 8272, 8623, 8542, 8524,8425, 8353, 8443, 832222, 823222, 822322, 7732, 7624, 7462, 7633, 7363, 7552, 7525, 7534, 7453, 724222, 733222, 732232, 723322, 723232, 6562, 6643, 6463, 6535, 6544, 652222, 625222, 622522, 634222, 632422, 632242, 632224, 642322, 623242, 624322, 623233, 623332, 632323, 5554, 553222, 525223, 522523, 522253, 552232, 525232, 542422, 542224, 524242, 543322, 543223, 542332, 542323, 542233, 534232, 533422, 533242, 532432, 532423, 524332, 533323, 444322, 424423, 442243, 424243, 443332, 433432, 443323, 434323, 433333, 43222222, 42232222, 33322222, 33232222, 33223222, 32232232
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caused by the extremely large number of possible layer sequences of high-layered polytypes.

In part 2, the author illustrates how successfully the simplified method works for actual cases of determination of SiC polytypes $20H_{(a)}$ and $20H_{(b)}$.

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