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Crystal Structures of Six New Polytypes of Cadmium Iodide

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Crystal structures of six newly discovered polytypes, $16H_4$, $18H_4$, $28H_2$, $28H_3$, $36H_1$ and $40H_1$, have been determined. The structures are represented by $(22)_3 1111$, (222122121111), $(22)_4 11222211$, $(22)_5 112211$, $(22221111)_2 11112222$ and $(22)_7 21122211$ in Zhdanov symbols. They all belong to the space group $P3m1$. The two cell dimensions, $a=b=4{\cdot}24$ Å, are identical for all the polytypes while the c dimensions are 54·68, 61·52, 95·69, 123·03 and 136·70 Å for the polytypes, $16H_4$, $18H_4$, $28H_2$ or $28H_3$, $36H_1$ and $40H_1$, respectively. All six polytypes were found to have grown in syntactic coalescence with other polytypes, showing a transformation of structure during growth. To date, polytype $40H_1$ is the largest hexagonal cadmium iodide polytype for which the structure has been determined. The mode of growth of these polytypes is discussed.

During the course of study of polytype growth in cadmium iodide crystals by successively cleaving the crystals parallel to their basal plane (Gyaneshwar & Trigunayat, 1972), six new polytypes have been discovered, for which it has been possible to determine the complete crystal structures. The crystals show structural transformation during growth and provide information regarding the process of polytype formation and the role played by the stacking faults therein.

Experimental methods

The crystals were grown from solution. A suitable range of oscillation, *viz.* the one in which the angle between the incident beam and the c axis varied between 25 and 40°, was chosen to record a large succession of 10.l reflexions on the X-ray film (Chadha & Trigunayat, 1967). These reflexions were employed to compare the calculated intensities with those observed, for structure analysis.

Structure of polytypes

(i) *Polytype* $16H_4$*

This polytype [Fig. 1(*a*)] was discovered in a well developed thin crystal. It occurred in syntactic coalescense with the common type 4H. Three other 16-layered polytypes have already been reported (Lal, Chadha & Trigunayat, 1971). Although a stupendously vast number of possiblities exist for such a large unit cell, nevertheless the task of postulating the correct crystal structure was facilitated by the observation that the intensity sequence of 10.l spots closely simulated those of known polytypes of the series $(22)_n 1111$. Four members of this series, *viz.* (22)1111, $(22)_2 1111$, $(22)_4 1111$ and $(22)_6 1111$, have been reported earlier. Thus the possible structure of the present polytype could be $(22)_3 1111$. The intensity calculations were made for the

* The polytype representation in this paper follows the scheme of notation suggested by Trigunayat & Chadha (1971)

10.*l* reflexions, with *l* varying from 0 to 32, using the formulae,

$$I = A^2 + B^2 \qquad (1)$$

where,

$$A = [\sum_{zA,\alpha} f_{I,Cd} \cos 2\pi lz + \sum_{zB,\beta} f_{I,Cd} \cos 2\pi(lz - \tfrac{1}{3}) + \sum_{zC,\gamma} f_{I,Cd} \cos 2\pi(lz + \tfrac{1}{3})]$$

and

$$B = [\sum_{zA,\alpha} f_{I,Cd} \sin 2\pi lz + \sum_{zB,\beta} f_{I,Cd} \sin 2\pi(lz - \tfrac{1}{3}) + \sum_{zC,\gamma} f_{I,Cd} \sin 2\pi(lz + \tfrac{1}{3}) .$$

$z_{A,\alpha}$, $z_{B,\beta}$ and $z_{C,\gamma}$ denote the respective z coordinates of the iodine (italic letters) and cadmium (Greek letters) atoms on the vertical A, B and C axes, respectively. $\sum_{zA,\alpha}$ represents summation over iodine atoms at A sites and cadmium atoms at α sites, and likewise for the other two summations. The intensities obtained by employing expression (1) were multiplied by the Lorentz–polarization factor $(1+\cos^2 2\theta)/\sin 2\theta$. The calculated intensities for the postulated structure are listed in Table 1(*a*). An excellent agreement exists between the calculated and the observed intensities.

The detailed structure of $16H_4$ is as follows: Zhdanov symbol $(22)_3 1111$

ABC sequence

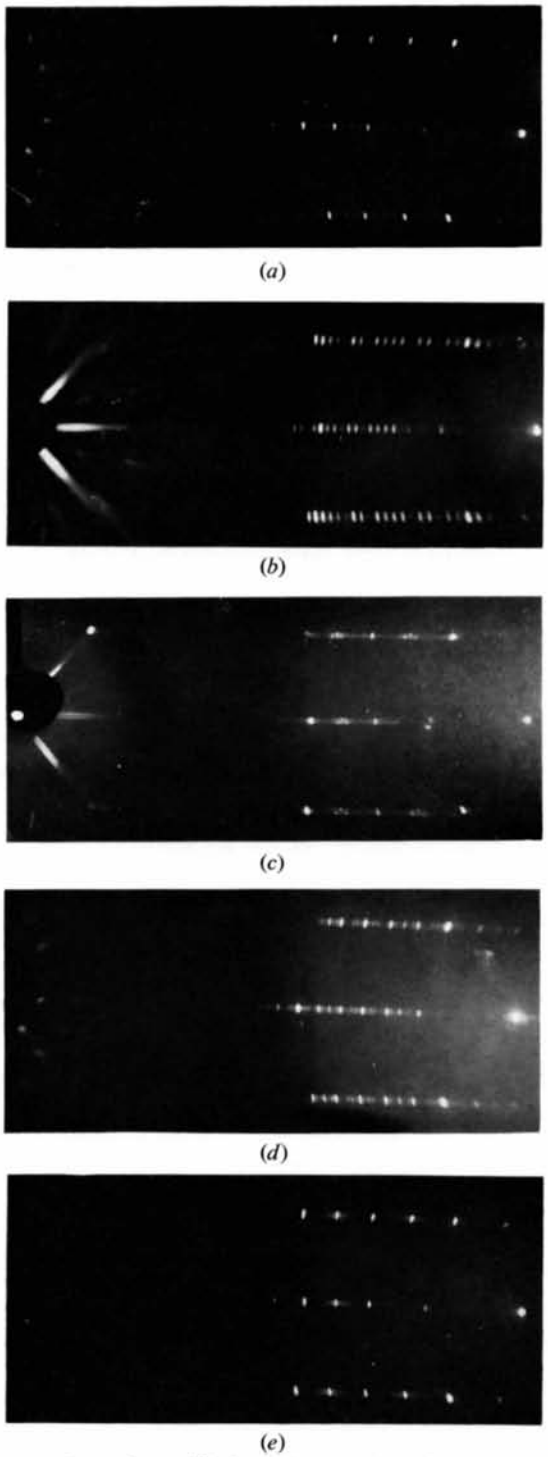
$(A\gamma B)\,(C\alpha B)\,(A\gamma B)\,(C\alpha B)\,(A\gamma B)\,(C\alpha B)\,(A\gamma B)\,(A\gamma B)$

Atomic coordinates

Iodine atoms at $00n_1z$, $\frac{2}{3}\frac{1}{3}n_2z$, $\frac{1}{3}\frac{2}{3}n_3z$; $n_1 = 0, 8, 16, 24, 28$; $n_2 = 2, 6, 10, 14, 18, 22, 26, 30$ and $n_3 = 4, 12, 20$.

Table 1. *Observed and calculated relative intensities for* 10.*l reflexions of polytypes* $16H_4$, $18H_4$, $28H_2$, $28H_3$, $36H_1$ *and* $40H_1$

l	Observed* intensity	Calculated intensity	*l*	Observed intensity	Calculated intensity	*l*	Observed intensity	Calculated intensity
(*a*) $16H_4$								
4	*ms*	78	11	*w*	34	18	*w*	27
5	*vw*	12	12	*vs*	317	19	*w*	24
6	*vw*	17	13	*w*	35	20	*ms*	194
7	*vw*	21	14	*w*	35	21	*vw*	18
8	*vvs*	527	15	*w*	34	22	*vw*	15
9	*w*	29	16	*s*	206	23	*vw*	12
10	*w*	31	17	*w*	30	24	*vs*	384
(*b*) $18H_4$								
4	*vvw*	7	13	*s*	386	22	*s*	308
5	*ms*	151	14	*s*	292	23	*vw*	16
6	*ms*	99	15	*vw*	22	24	*w*	40
7	*vw*	19	16	*s*	307	25	*ms*	126
8	*ms*	124	17	*s*	230	26	*s*	247
9	*vvs*	1621	18	*s*	206	27	*vs*	555
10	*ms*	120	19	*s*	270	28	*ms*	164
11	*s*	214	20	*vvw*	6			
12	*w*	63	21	*s*	204			
(*c*) $28H_2$								
8	*w*	66	20	*s*	216	32	*a*	1
9	*vvw*	16	21	*ms*	54	33	*vw*	32
10	*a*	0	22	*s*	225	34	*s*	152
11	*a*	10	23	*w*	44	35	*vw*	34
12	*a*	3	24	*a*	1	36	*s*	129
13	*a*	1	25	*vvw*	21	37	*vvw*	23
14	*vvs*	698	26	*a*	6	38	*a*	0
15	*a*	2	27	*a*	2	39	*a*	9
16	*a*	5	28	*s*	221	40	*a*	2
17	*vvw*	18	29	*a*	2	41	*a*	0
18	*a*	1	30	*a*	5	42	*vs*	420
19	*w*	41	31	*vvw*	17			
(*d*) $28H_3$								
7	*w*	51	19	*w*	64	31	*a*	3
8	*vw*	32	20	*ms*	103	32	*a*	22
9	*vvw*	25	21	*s*	216	33	*w*	50
10	*a*	12	22	*ms*	108	34	*w*	72
11	*a*	2	23	*w*	69	35	*ms*	137
12	*a*	0	24	*vvw*	28	36	*w*	62
13	*a*	5	25	*a*	4	37	*vw*	36
14	*vvs*	698	26	*a*	0	38	*a*	13
15	*a*	6	27	*a*	8	39	*a*	1
16	*a*	0	28	*s*	221	40	*a*	0
17	*a*	3	29	*a*	7	41	*a*	2
18	*vvw*	25	30	*a*	0	42	*vs*	420



(*a*)

(*b*)

(*c*)

(*d*)

(*e*)

Fig. 1. 15° *a*-axis oscillation photographs of the polytypes (*a*) $16H_4$, (*b*) $18H_4$, (*c*) $28H_2$ and $28H_3$, (*d*) $36H_1$ and (*e*) $40H_1$; 3 cm camera; Cu $K\alpha$ radiation. The strongest spot on the zero layer line in each case has the index $10.n/2$, where n is the number of layers in the unit cell of the polytype.

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Table 1 (*cont.*)

l	Observed* intensity	Calculated intensity	*l*	Observed intensity	Calculated intensity	*l*	Observed intensity	Calculated intensity
(*e*) $36H_1$								
10	*vvw*	3	25	*ms*	23	40	*a*	2
11	*vvw*	8	26	*vw*	10	41	*a*	2
12	(*vs*)†	7	27	*s*	223	42	(*vs*)	13
13	*a*	1	28	*vw*	10	43	*ms*	16
14	*a*	1	29	*ms*	24	44	*vvw*	6
15	*vw*	10	30	(*vs*)	18	45	*s*	137
16	*w*	15	31	*a*	2	46	*vvw*	5
17	*vvw*	6	32	*a*	2	47	*w*	12
18	*vvs*	417	33	*ms*	18	48	(*vs*)	9
19	*vvw*	7	34	*ms*	23	49	*a*	1
20	*ms*	19	35	*vvw*	9	50	*a*	1
21	*w*	15	36	(*vs*)	206	51	*vvw*	7
22	*a*	2	37	*vvw*	9	52	*vvw*	8
23	*a*	2	38	*ms*	20	53	*a*	3
24	(*vs*)	17	39	*w*	15	54	(*vs*)	376
(*f*) $40H_1$								
8	*vvw*	10	14	*a*	2	20	*vvs*	839
9	*w*	19	15	*a*	0	21	*a*	1
10	*ms*	59	16	*a*	1	22	*a*	5
11	*w*	27	17	*a*	4	23	*a*	6
12	*vw*	21	18	*a*	4	24	*a*	2
13	*vvw*	11	19	*a*	1	25	*a*	0
26	*a*	5	38	*a*	5	50	*s*	128
27	*w*	26	39	*a*	2	51	*ms*	47
28	*ms*	57	40	*vs*	184	52	*w*	29
29	*s*	87	41	*a*	1	53	*vw*	12
30	*vs*	224	42	*a*	5	54	*a*	2
31	*s*	88	43	*a*	5	55	*a*	0
32	*ms*	59	44	*a*	2	56	*a*	1
33	*w*	27	45	*a*	0	57	*a*	2
34	*a*	6	46	*a*	4	58	*a*	1
35	*a*	0	47	*vw*	18	59	*a*	0
36	*a*	3	48	*w*	37	60	*vs*	285
37	*a*	6	49	*ms*	53			

* The observed intensities were actually taken from the series $10.2n$ to $10.4n$ which have a similar sequence to the series 10.0 to $10.2n$ ($n=16$, 18, 28, 36, 40 for the polytypes $16H_4$, $18H_4$, $28H_2$ or $28H_3$, $36H_1$ and $40H_1$, respectively).

† The reflexion in parentheses could not be well resolved owing to its overlapping with the $6H$ spots.

Cadmium atoms at $00n_4z$, $\frac{1}{3}\frac{2}{3}n_5z$; $n_4=5,13,21$; $n_5=1,9,17,25,29$ where $z=\frac{1}{3}\frac{1}{2}$.

(ii) *Polytype* $18H_4$

This well ordered polytype was discovered on the upper face of a crystal, which had its lower face in contact with the bottom of the crystallizing dish at the time of growth. The lower face of the crystal was found to be an unidentified disordered high polytype. A close examination of the intensity sequence of the spots revealed that it was not symmetrical and that it resembled the intensity sequence of the common type $4H$ [structure (22)] [Fig. 1(*b*)]. This, in turn, implied that the Zhdanov sequence of the structure was, most likely, unsymmetrical, and that it consisted of many (22) units. Consequently, we were led to formulate the following structures as the probable ones:

(1) 222122111111
(2) 222122211111
(3) 222122121111
(4) 222112122111
(5) 222111121221

The intensities for the $10.l$ reflexions were computed for each of the structures proposed above. Excellent agreement between the calculated [Table 1(*b*)] and observed values was found for the case of structure (3). The crystal structures of three 18-layered cadmium iodide polytypes have already been reported by different workers. Thus the present polytype was designated as $18H_4$. The detailed structure of the polytype is:

Zhdanov symbol 222122121111

ABC sequence

$(A\gamma B)$ $(C\alpha B)$ $(A\gamma B)$ $(C\alpha B)$ $(C\beta A)$ $(C\alpha B)$ $(C\alpha B)$ $(A\gamma B)$ $(A\gamma B)$

Atomic coordinates

Iodine atoms at $00n_1z$, $\frac{2}{3}\frac{1}{3}n_2z$, $\frac{1}{3}\frac{2}{3}n_3z$; $n_1=0,8,18,28,32$; $n_2=2,6,10,14,22,26,30,34$; $n_3=4,12,16,20,24$.

Cadmium atoms at $00n_4z$, $\frac{2}{3}\frac{1}{3}n_5z$, $\frac{1}{3}\frac{2}{3}n_6z$; $n_4=5,13,21,25$; $n_5=17$; $n_6=1,9,29,33$.

where $z=\frac{1}{3}\frac{1}{6}$.

(iii) *Polytypes* $28H_2$ *and* $28H_3$

These two polytypes of the same *c* dimension but

different crystal structures were found to coexist on the upper face of a crystal. In the region of reflexion, corresponding to the upper face of the crystal, each layer line on the oscillation photograph was found to consist of two parallel rows of spots, which had the same spacing, but different sequences of intensity [Fig. 1(*c*)]. Since the crystal structure of a 28-layered polytype has been already determined (Trigunayat & Chadha, 1971), these two polytypes pertaining to the lower and upper rows of spots in Fig. 1(*c*), were labelled as $28H_2$ and $28H_3$, respectively. The lower face of the crystal was detected as the polytype $52H$, with heavy streaking along the layer lines.

As seen in Fig. 1(*c*), for both the polytypes, the intense spots were found to be either coinciding with or lying around the positions of reflexions of the common type $4H$, which indicated that both structures were based on $4H$. This led to the postulation of the following structures:

(1) $(22)_5211211$
(2) $(22)_5112211$
(3) $(22)_421122211$
(4) $(22)_411222211$
(5) $(22)_32112222211$.

Of these, the calculated values of intensities for structures (2) and (4) were found to be in excellent agreement with the observed values for the polytypes $28H_2$ and $28H_3$, respectively [Table 1(*c*) and (*d*)].

The detailed structure of $28H_2$ is:
Zhdanov symbol $(22)_411222211$
ABC sequence
$(A\gamma B)$ $(C\alpha B)$ $(A\gamma B)$ $(C\alpha B)$ $(A\gamma B)$ $(C\alpha B)$ $(A\gamma B)$ $(C\alpha B)$ $(A\gamma B)$ $(A\gamma B)$ $(C\alpha B)$ $(A\gamma B)$ $(C\alpha B)$ $(A\gamma B)$
Atomic coordinates:
Iodine atoms at $00n_1z$, $\frac{2}{3}\frac{1}{3}n_2z$, $\frac{1}{3}\frac{2}{3}n_3z$; $n_1=0, 8, 16, 24, 32, 36, 44, 52$; $n_2=2, 6, 10, 14, 18, 22, 26, 30, 34, 38, 42, 46, 50, 54$; $n_3=4, 12, 20, 28, 40, 48$.
Cadmium atoms at $00n_4z$, $\frac{1}{3}\frac{2}{3}n_5z$; $n_4=5, 13, 21, 29, 41, 49$; $n_5=1, 9, 17, 25, 33, 37, 45, 53$.
where $z=\frac{1}{56}$.

The detailed structure of $28H_3$ is as follows:
Zhdanov symbol $(22)_5112211$
ABC sequence
$(A\gamma B)$ $(C\alpha B)$ $(A\gamma B)$ $(C\alpha B)$ $(A\gamma B)$ $(C\alpha B)$ $(A\gamma B)$ $(C\alpha B)$ $(A\gamma B)$ $(C\alpha B)$ $(A\gamma B)$ $(A\gamma B)$ $(C\alpha B)$ $(A\gamma B)$
Iodine atoms at $00n_1z$, $\frac{2}{3}\frac{1}{3}n_2z$, $\frac{1}{3}\frac{2}{3}n_3z$; $n_1=0, 8, 16, 24, 32, 40, 44, 52$; $n_2=2, 6, 10, 14, 18, 22, 26, 30, 34, 38, 42, 46, 50, 54$; $n_3=4, 12, 20, 28, 36, 48$.
Cadmium atoms at $00n_4z$, $\frac{1}{3}\frac{2}{3}n_5z$; $n_4=5, 13, 21, 29, 37, 49$; $n_5=1, 9, 17, 25, 33, 41, 45, 53$.
where $z=\frac{1}{56}$.

(iv) *Polytype* $36H_1$

This new modification was discovered on the lower face of a well developed crystal [Fig. 1(*d*)]. The upper face of the crystal was identified as another 36-layered polytype, but with a completely different intensity sequence of reflexions. Since the crystal presented interesting structural transformation during growth, attempts were made to determine the structures of both these polytypes. However, owing to the dearth of necessary clues, the structure of the latter could not be ascertained. Regarding the former, its intense reflexions were found to lie at the positions of small period polytype $6H$ [structure (2211)] [Fig. 1(*d*)]. Hence a large number of structures consisting of several (2211) units were tried, but to no avail. The failure of these attempts made us to suspect that the structure could be based on a $12H$ polytype, instead of $6H$, because the alternate spots of $12H$ would lie at the positions of $6H$. On the basis of this conjecture the following structures were postulated (each postulated sequence consists of three $12H$ units):

(1) 112222111122221111112222
(2) 222211112222111222222
(3) 11222211112222111222222
(4) 222211112222211111112222
(5) 221122112222211111112222
(6) 2211112222222111111112222 .

Excellent agreement between the calculated and observed values of intensities, listed in Table 1(*e*), was obtained for structure (4). So far, 13 polytypes of 36 layers each have been reported by five different workers (Trigunayat & Chadha, 1971), but the crystal structure of none of them has been determined. Consequently, the present polytype was designated as $36H_1$.

The detailed structure of $36H_1$ is:
Zhdanov symbol $(22221111)_211112222$
ABC sequence
$(A\gamma B)$ $(C\alpha B)$ $(A\gamma B)$ $(C\alpha B)$ $(A\gamma B)$ $(A\gamma B)$ $(A\gamma B)$ $(C\alpha B)$ $(A\gamma B)$ $(C\alpha B)$ $(A\gamma B)$ $(A\gamma B)$ $(A\gamma B)$ $(A\gamma B)$ $(A\gamma B)$ $(C\alpha B)$ $(A\gamma B)$ $(C\alpha B)$
Atomic coordinates
Iodine atoms at $00n_1z$, $\frac{2}{3}\frac{1}{3}n_2z$, $\frac{1}{3}\frac{2}{3}n_3z$; $n_1=0, 8, 16, 20, 24, 32, 40, 44, 48, 52, 56, 64$; $n_2=2, 6, 10, 14, 18, 22, 26, 30, 34, 38, 42, 46, 50, 54, 58, 62, 66, 70$; $n_3=4, 12, 28, 36, 60, 68$.
Cadmium atoms at $00n_4z$, $\frac{1}{3}\frac{2}{3}n_5z$; $n_4=5, 13, 29, 37, 61, 69$; $n_5=1, 9, 17, 21, 25, 33, 41, 45, 49, 53, 57, 65$.
where $z=\frac{1}{72}$.

(v) *Polytype* $40H_1$

This new polytype was discovered on the lower face of a well developed crystal, the upper face of which was found to be the common type $4H$ [Fig. 1(*e*)]. Although initially the task of structure determination for such a large cell looked prohibitively difficult, a very useful indication was obtained from the observation that the intense diffraction spots of this polytype coincided with and lay around the alternate positions of $4H$ reflexions. Therefore a very large number of structures consisting of many (22) units, were postulated. The structure corresponding to the Zhdanov sequence $(22)_721122211$ gave the best match between the observed and calculated intensities [Table 1(*f*)].

The detailed structure of $40H_1$ is:

Zhdanov symbol $(22)_7 21122211$

ABC sequence

$(A\gamma B)\ (C\alpha B)\ (A\gamma B)\ (C\alpha B)\ (A\gamma B)\ (C\alpha B)\ (A\gamma B)\ (C\alpha B)$
$(A\gamma B)\ (C\alpha B)\ (A\gamma B)\ (C\alpha B)\ (A\gamma B)\ (C\alpha B)\ (A\gamma B)\ (C\alpha B)$
$(C\alpha B)\ (A\gamma B)\ (C\alpha B)\ (A\gamma B)$

Atomic coordinates

Iodine atoms at $00n_1z$, $\frac{2}{3}\frac{1}{3}n_2z$, $\frac{1}{3}\frac{2}{3}n_3z$; $n_1=0, 8, 16, 24, 32, 40, 48, 56, 68, 76$; $n_2=2, 6, 10, 14, 18, 22, 26, 30, 34, 38, 42, 46, 50, 54, 58, 62, 66, 70, 74, 78$; $n_3=4, 12, 20, 28, 36, 44, 52, 60, 64, 72$.

Cadmium atoms at $00n_4z$, $\frac{1}{3}\frac{2}{3}n_5z$; $n_4=5, 13, 21, 29, 37, 45, 53, 61, 65, 73$; $n_5=1, 9, 17, 25, 33, 41, 49, 57, 69, 77$.

where $z=\frac{1}{80}$.

Discussion

Recent studies in polytypic crystals have shown that stacking faults play an important role in the growth of polytypes (Trigunayat, 1971). The stacking faults constitute departure from the normal sequence of stacking of layers in a crystal. Much earlier, Jagodzinski (1954*a*) had visualized a physical mechanism of the formation of SiC polytypes by the introduction of suitable stacking faults in the crystal structure of the common SiC type $6H$. The strongly anisotropic nature of the crystal structure of cadmium iodide renders it specially favourable for the generation of stacking faults, by mutual slippage of layers parallel to the basal plane (Agrawal & Trigunayat, 1969). Judging from the vast abundance of the common CdI_2 type $4H$, it can be safely assumed that the growth of all cadmium iodide crystals starts as $4H$, which, under appropriate conditions may later transform into another polytype. Thus the growth of the polytypes $16H_4$, $36H_1$ and $40H_1$, of which the crystal structures have been determined by us and which have all been detected on the lower crystal faces, could possibly result from the introduction of stacking faults in the basic type $4H$. However, the existence of three successive 12-layered units in the crystal structure of polytype $36H_1$ indicates that the polytype $12H$ must have first been formed from $4H$ in the initial stages of crystal growth and later transformed into the polytype $36H_1$ by suitable layer displacements. Thus, starting from the common type $4H$, with crystal structure as *ABCBABCB* ...in Zhdanov notation, the most probable schemes of layer transposition operative in the formation of the polytypes $16H_4$, $36H_1$ and $40H_1$ should be the following:

$16H_4$

ABCBABCBABCBABCB $(4H)$

↓

ABCBABCBABCBABAB $(16H_4)$

$36H_1$

ABCBABCBABCB $(4H)$

↓

ABCBABCBABAB $(12H)$

ABCBABCBABABABCBABCBABABABCBABCBABAB $(12H)$

↓ ↓

ABCBABCBABABABCBABCBABABABABABCBABCB $(36H_1)$

$40H_1$

ABCBABCBABCBABCBABCBABCBABCBABCBABCBABCB $(4H)$

↓ ↓ ↓ ↓

ABCBABCBABCBABCBABCBABCBABCBABCBCBABCBAB $(40H_1)$

The above schemes of polytype formation involve minimum numbers of layer displacements and therefore, should be energetically most favourable.

The modes of transformation for the other three polytypes, $18H_4$, $28H_2$ and $28H_3$, each detected at upper face, cannot be visualized, as structures of the respective polytypes on the lower face of the crystals have remained unknown. Nevertheless, the polytype $18H_4$ has been transformed from a disordered high polytype (unidentified) and the other two polytypes, $28H_2$ and $28H_3$, also show the transformation of structure from a disordered $52H$ polytype. The presence of disorder was revealed from the existence of heavy streaking of reflexions on the oscillation photographs (not reproduced), obtained from the lower faces of the respective crystals. Since such disorder essentially stems from a random distribution of stacking faults (Shaw, Steadman & Pugh, 1965) in the structure, it imparts instability to the structure. Hence, from a thermodynamic point of view, there should be a natural tendency for the structure to pass over into a stable one, presumably through appropriate layer transpositions.

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