intensities for polytypes and specific shape of the diffuse streaks (broadened $10.l$ reflexions) for disordered structures are closely connected with the type of faulting occurring in the crystals (Pałosz, 1980*b*). Based on this it seems possible to determine directly the type and degree of faulting for disordered structures: in this case the experimentally observed intensity curves should be compared with the $10.l/10.\bar{l}$ reflexion intensities calculated for structural models. A similar procedure was earlier applied to identify disordered structures of ZnS (Pałosz, 1977), and is now being extensively investigated for its possible use with disordered MX_2 structures.

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Atomic Positions of Three New Polytypes of CdI_2

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Abstract

The crystal structures of three new polytypes $16H_9$, $24H_8$ and $44H_1$ of cadmium iodide have been determined. The structures are $22(11)_6$, $2222(211211)_2$ and $(22211211)(121121)_4$ in Zhdanov notation, each with space group $P3m1$. All three polytypes have been found syntactically coalesced with other polytypes in three different crystals. Polytype $44H_1$ is the largest hexagonal polytype of cadmium iodide whose structure has been reported so far.

Introduction

Extensive work during the last two decades has resulted in the discovery not only of many new polytypes of known substances but also of many new polytypic substances. Not only do these discoveries help in understanding the phenomenon of polytypism more clearly but many new fields, like interpolytypic, intrapolytypic, phase transformation (Tewari & Srivastava, 1974), dielectric behaviour of polytypes (Fernandez & Srivastava, 1975) and polytypes as a new class of variable band-gap materials (Rao & Srivastava, 1980), also develop side by side. Of late, many new techniques have been employed for investigating various aspects of polytypism (Trigunayat, 1981). Although much work has been done on polytypism the total number of CdI_2 polytypes with known structure is less than a hundred (Wahab & Trigunayat, 1980). Recently the structure-factor calculations of MX_2-type compounds have been simplified (Chadha, 1980) and, using this simplified structure-factor formula, the largest hexagonal structure of CdI_2 ($44H$) to be determined so far is presented here. Besides this, two other structures, $16H$ and $24H$, have also been determined.

Experimental methods and structure determination

Good hexagonal platy crystals, measuring 1–2 mm across and having a thickness of about 100 μm grown

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by the evaporation of an aqueous solution, were used in the present study. The method of growth, the selection of crystals, and the suitable range of oscillation photographs have been described in previous publications (*e.g.* Chadha & Trigunayat, 1967*a*).

The 10.*l* reflexions are sufficient for a complete structure analysis of polytypic crystals. The intensities of these reflections are calculated using the expression (Chadha, 1980) $I_{10.l} \propto |F_{10.l}|^2$

where

$$F_{10.l} = \{2f_1 \cos 2\pi|\tfrac{1}{3} + l/(2n)| + f_{Cd}\} \times \sum_{z_c=\text{clockwise}} \exp\{2\pi i|x_c + lz_c/(2n)|\} + \{2f_1 \cos 2\pi|-\tfrac{1}{3} + l/(2n)| + f_{Cd}\} \times \sum_{z_a=\text{anticlockwise}} \exp\{2\pi i|x_a + lz_a/(2n)|\}.$$

The expression does not contain any term for the summation of iodine atoms. Both the summations are over cadmium atoms in clockwise and anticlockwise types of sandwiches. The cadmium atoms in sandwiches of the type ($A\gamma B$), ($B\alpha C$) or ($C\beta A$) are used in the first summation, called clockwise, while ($B\gamma A$), ($C\alpha B$) or ($A\beta C$) are called anticlockwise sandwiches. The summation over the atoms has been replaced by summation over the z coordinates of cadmium atoms with the x coordinate taken as a function of z. x_c and x_a will be 0, $\frac{2}{3}$ or $\frac{1}{3}$ depending on whether the atom is in an α, β or γ orientation respectively for a certain value of z_c or z_a. The values of I for different l values, obtained from the above, are multiplied by the Lorentz–polarization factor $(1 + \cos^2\theta)/\sin 2\theta$, where θ is the Bragg angle.

Oscillation photographs for the three polytypes are shown in Fig. 1.

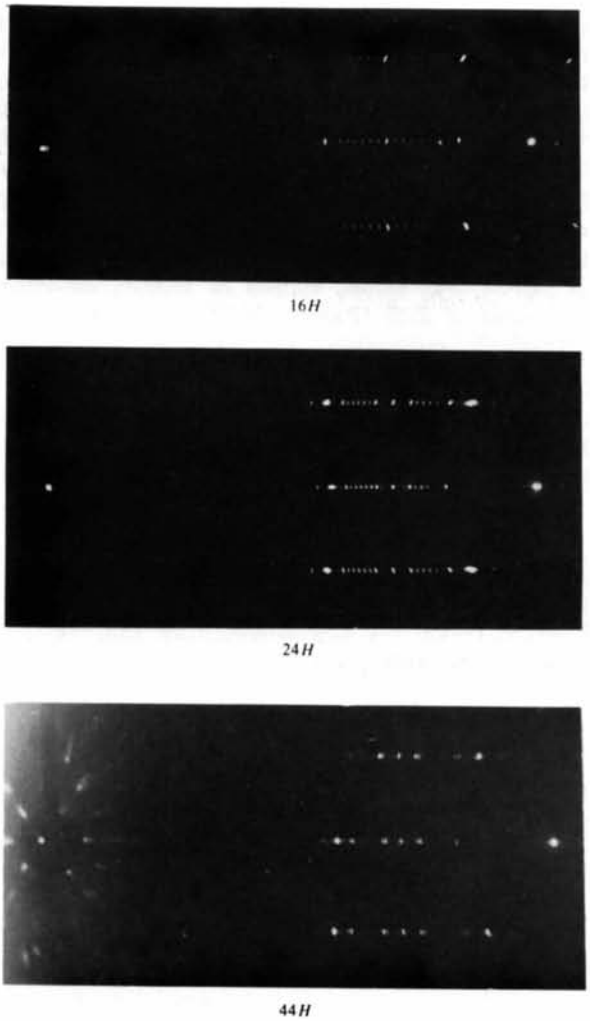

Fig. 1. 15° *a*-axis oscillation photograph of 16*H*, 24*H* and 44*H* polytypes (3 cm camera; Cu $K\alpha$ radiation). The first most intense spot from the centre on the zero layer has $l = 5n/2$ for all the three *nH* polytypes.

Polytype 16*H*

This polytype, $16H_9$, is found in a crystal coalesced with 2*H*. Therefore, it is expected that the crystal has grown from one with the basic structure 2*H*(11). Moreover, the intensities observed in the X-ray photograph show a similarity to 2*H* as the strongest reflections coincide with 2*H* reflections. Therefore, it was expected that the crystal should contain a large number of (11) units. Various arrangements containing a large number of (11) units were tried and the calculated intensities were compared with the observed values. Excellent agreement was obtained for the structure $22(11)_6$ listed in Table 1.

The detailed structure of $16H_9$ is therefore as follows: cell dimensions: $a = b = 4{\cdot}24$, $c = 54{\cdot}68$ Å; space group: $P3m1$; *ABC* sequence:

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

Table 1. *Calculated and observed relative intensities for* 10.*l reflections of the polytype* $16H_9$

The strong reflections in the photograph have increasing intensities from $l = 35$ to 47 and from $l = 57$ to 49.

10.*l*	Observed intensity	Calculated intensity	10.*l*	Observed intensity	Calculated intensity
35	w	13	48	vvs	1290
36	s	22	49	s	88
37	s	31	50	s	84
38	s	40	51	s	79
39	s	50	52	s	74
40	vvs	629	53	s	68
41	s	68	54	s	61
42	s	75	55	s	53
43	s	81	56	vvs	2988
44	s	86	57	s	38
45	s	89			
46	s	91			
47	s	91			

Atomic coordinates used for summations: (i) clockwise: $[\frac{1}{3},\frac{2}{3},z_c/(2n)]$, z_c = 1, 9, 13, 17, 21, 25, 29; (ii) anticlockwise: $[0,0,5/(2n)]$.

Polytype 24*H*

Polytype $24H_8$ was found to be syntactically coalesced with another polytype 24*H*. The intensity distribution of the second 24*H* type was very unsymmetric and we therefore did not try to determine its structure. The X-ray reflections for $24H_8$ were found to be quite symmetrical. The most intense spots coincided with either 4*H* or 8*H* spots. The intensity distribution of 8*H* spots seemed to be of the type (211211) structure (Chadha & Trigunayat, 1967*b*). Therefore, we tried the various combinations of 22 and 211211 to obtain the required $24H_8$ intensities. The best agreement was obtained for a structure $2222(211211)_2$, as can be seen in Table 2.

The detailed structure of $24H_8$ is therefore as follows: cell dimensions: $a = b = 4{\cdot}24$, $c = 82{\cdot}02$ Å; space group: $P3m1$; *ABC* sequence:

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

Atomic coordinates used for summations: (i) clockwise: $[\frac{1}{3},\frac{2}{3},z_c/(2n)]$; z_c = 1, 9, 17, 29, 33, 45; (ii) anticlockwise: $[0,0,z_a/(2n)]$; z_a = 5, 13, 21, 25, 37, 41.

Polytype 44*H*

Polytype 44*H* is syntactically coalesced with an unidentified polytype on the other side of the crystal. The lattice height of the crystal is a multiple of 4*H*, but the intensity distribution of the 10.*l* reflections seems to favour 2*H*. Therefore we assumed various combinations of 2*H* and 4*H* in the structure, but could not obtain the required intensity distribution. On further examination we found that some of the strong reflections lie near 8*H* reflection positions. The 8*H* structure which has this intensity distribution has the (121121) Zhdanov notation. Therefore we postulated different structures having configurations of the type $(121121)_n(22)_m$, $(121121)_n(11)_m$ or $(121121)_n(22)_m(11)_p$ with different values of *n*, *m* and *p*. Excellent agreement was obtained for the structure $22211211(121121)_4$ (Table 3). The detailed structure of $44H_1$ is as follows: cell dimensions: $a = b = 4{\cdot}24$, $c = 150{\cdot}37$ Å; Zhdanov symbol: $22211211(121121)_4$; space group: $P3m1$; *ABC* sequence:

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

Atomic coordinates: (i) clockwise: $[\frac{1}{3},\frac{2}{3},z_c/(2n)]$; z_c = 1, 9, 21, 25, 37, 41, 53, 57, 69, 73, 85; (ii) anticlockwise: $[0,0,z_a/(2n)]$; z_a = 5, 13, 17; $[\frac{2}{3},\frac{1}{3},z_a/(2n)]$; z_a = 29, 33, 45, 49, 61, 65, 77, 81.

Table 2. *Calculated and observed relative intensities for* 10.*l reflections of the polytype* $24H_8$

As there are better reflections on the first layer (01.*l*), the intensities were observed on this layer.

10.*l*	Observed intensity	Calculated intensity	10.*l*	Observed intensity	Calculated intensity
50	*a*	0·47	69	*vs*	251·0
51	*vw*	8·3	70	*w*	32·0
52	*vw*	5·7	71	*vw*	8·7
53	*w*	11·3	72	*vs*	391·71
54	*w*	17·6	73	*vw*	8·7
55	*w*	22·5	74	*w*	32·25
56	*w*	23·5	75	*vs*	253·8
57	*s*	78·7	76	*s*	92·9
58	*w*	11·9	77	*s*	112·1
59	*vw*	3·8	78	*s*	115·4
60	*vvs*	1067·7	79	*s*	102·6
61	*vw*	4·9	80	*s*	78·0
62	*w*	20·7	81	*vs*	194·89
63	*vs*	181·7	82	*w*	22·6
64	*s*	73·9	83	*vw*	5·54
65	*s*	98·5	84	*vvs*	1240·56
66	*s*	111·8			
67	*s*	109·4			
68	*s*	91·4			

Table 3. *Calculated and observed relative intensities for* 10.*l reflections of the polytype* $44H_1$

10.*l*	Observed intensity	Calculated intensity	10.*l*	Observed intensity	Calculated intensity
106	2	*vw*	124	37·7	*w*
107	29·9	*w*	125	20·3	*w*
108	97·3	*s*	126	124·3	*vs*
109	167·9	*s*	127	274·6	*vs*
110	760·3	*vvs*	128	16·5	*w*
111	185·1	*s*	129	15·3	*w*
112	119·1	*s*	130	45·8	*ms*
113	42·1	*w*	131	73·8	*s*
114	2	*vw*	132	146·8	*vs*
115	161·8	*vs*	133	66·6	*ms*
116	143·7	*vs*	134	40·6	*ms*
117	22·1	*w*	135	16·9	*w*
118	26·4	*w*	136	9·0	*w*
119	20·0	*w*	137	151·7	*vs*
120	9·2	*w*	138	252·5	*vs*
121	8·6	*w*	139	34·9	*w*
122	21·8	*w*	140	13·6	*bw*
123	37·1	*w*	141	7·7	*vs*

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