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Structures of 21 New Polytypes of Cadmium Iodide

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Abstract. The structures of 21 new polytypes of CdI_2 obtained from solutions are presented: 4 hexagonal polytypes: $12H_{10}$: $f5tf4f2of1$; $16H_{11}$: $tf5tf4(f2f1)_2$; $20H_{15}$: $(tf2f1)_2tf2of1$; $22H_9$: $f5f1f1f5f1of1f2f2f1f1$; and 17 rhombohedral polytypes: $36R_8$: $tf5f4f2of1$; $36R_9$: $f5f4f2of2f4$; $42R_4$: $f2f2f4f2of1t$; $42R_5$: $f5f1of1f2f1t$; $42R_6$ $f2(o)_2f2f4(t)_2$; $48R_6$: $f5f1f1(t)_2f2f1t$; $48R_7$: $f5(t)_2f1f1f2f1t$; $54R_8$: $f2f2f1f1(t)_3f2f1$; $60R_4$: $f5f1f1f5f1(o)_4f1$; $60R_5$: $f5f1(o)_2f1f2f1(t)_3$; $60R_6$: $f5f1f1tf2f1tf2of1$; $66R_4$: $f2f2f1of1(t)_6$; $66R_5$: $f2of2f4f2(o)_2f1(t)_3$; $66R_6$: $(f5f1f1)_2f2f1f2of1$; $66R_7$: $f5f1f1f5f1f2f1f1f2of1$; $84R_6$: $f2of2f4(t)_4f2(o)_3f1t$; $108R_2$: $f5f4f5(t)_{11}f4(t)_3$.

Experimental. The crystals of CdI_2 were grown from alcoholic solutions by slow evaporation at room temperature (Gierlotka & Pałosz, 1983). They were examined by X-rays in a cylindrical camera with a 43 mm radius and 0·7 mm collimator. The a^*-axis oscillations were used with the angle between the incident beam (Ni-filtered Cu K radiation) and the c axis varying between 21 and 36° (Pałosz & Gierlotka, 1984). The intensities of $10.l$ and $1\bar{1}.l$ reflections (they correspond to $10.l$ and $10.\bar{l}$ reflections used earlier: Pałosz & Gierlotka, 1984) were measured on the patterns and compared with the values computed from the formula commonly used for CdI_2 crystals (Jain & Trigunayat, 1978). The diagrams presented in Figs. 1–21 compare the measured and calculated intensities for $10.l$ and $1\bar{1}.l$ reflections in the range $2{\cdot}5 \leq l/N \leq 3{\cdot}5$, were N is the number of iodine layers in a polytype cell.†

The identification of polytypes was based on the division of polytypes into structural series and into groups of symmetry of the patterns (Pałosz, 1982). To construct the structural models of the polytypes under investigation the rules of construction of the cells found earlier were used (Pałosz, 1983*a*).

Discussion. The structures of 21 new polytypes of CdI_2 are given in Table 1 where the sequences of *t–o–f* layers in the cells are presented. In this table the growth conditions for the polytypes identified are also given. The Zhdanov symbols corresponding to these *t–o–f* sequences are given in Figs. 1–21.

† Oscillation diagrams and digital data may be obtained on request.

Table 1. *Structure and growth conditions of* 21 *new polytypes of* CdI_2

Ramsdell* symbol	*t–o–f* notation of a cell	Solvent†	Series
Hexagonal polytypes			
$12H_{10}$	$f5tf4f2of1$	ia	SII/SIII-1
$16H_{11}$	$tf5tf4(f2f1)_2$	pr + aq = 1:1	SI/SIII-1
$20H_{15}$	$(tf2f1)_2tf2of1$	ia	$(S\text{II})_3$
$22H_9$	$f5f1f1f5f1of1f2f2f1f1$	ia	$(S\text{IV-4})_2/S\text{IV-2}$
Rhombohedral polytypes			
$36R_8$	$tf5f4f2of1$	ia	SII/SIV-I
$36R_9$	$f5f4f2of2f4$	ia	SIV-1/SIV-3
$42R_4$	$f2f2f4f2of1t$	ia	SIV-3/SII
$42R_5$‡	$f5f1of1f2f1t$	aq	SIV-2/SII
$42R_6$	$f2(o)_2f2f4(t)_2$	et	SIV-3
$48R_6$‡	$f5f1f1(t)_2f2f1t$	aq	SIV-2/SII
$48R_7$	$f5(t)_2f1f1f2f1t$	pr + aq = 1:1	SIV-4/SII
$54R_8$§	$f2f2f1f1(t)_3f2f1$	aq	SIV-2/SII
$60R_4$	$f5f1f1f5f1(o)_4f1$	ib + aq = 1:1	$(S\text{IV-4})_2$
$60R_5$	$f5f1(o)_2f1f2f1(t)_3$	ia	SIV-4/SII
$60R_6$	$f5f1f1tf2f1tf2of1$	ia	$S\text{IV-4}/(S\text{II})_2$
$66R_4$	$f2f2f1of1(t)_6$	et	SIV-2
$66R_5$	$f2of2f4f2(o)_2f1(t)_3$	ib + aq = 1:1	SIV-3/SII
$66R_6$	$(f5f1f1)_2f2f1f2of1$	ia	$(S\text{IV-4})_2/S\text{IV-2}$
$66R_7$	$f5f1f1f5f1f2f1f1f2of1$	ia	$(S\text{IV-4})_2/S\text{I}$
$84R_6$§	$f2of2f4(t)_4f2(o)_3f1t$	et + aq = 1:3	SIV-3/SII
$108R_2$‡	$f5f4f5(t)_{11}f4(t)_3$	et + aq = 1:1	SIV-1/SIII-I

* The indices of Ramsdell symbols are after Chadha (1982), Chaudhary, Chadha & Trigunayat (1983), Pałosz (1983*a,b,c*), Pałosz & Gierlotka (1984) and Gierlotka & Pałosz (1984).

† aq = water; et = ethanol C_2H_5OH; pr = propanol $CH_3CH_2CH_2OH$; ib = isobutyl alcohol (2-methylpropanol) $(CH_3)_2CHCH_2OH$; ia = isoamyl alcohol (3-methyl-1-butanol) $(CH_3)_2CHCH_2CH_2OH$.

‡ Crystals obtained in an external electric field (Pałosz & Przedmojski, 1982*a*).

§ Crystals obtained in an external magnetic field (Pałosz & Przedmojski, 1982*b*).

As is well known, several different polytypes frequently occur on one face of a crystal. By now we have identified the structures of several series of hexagonal polytypes coexisting with other hexagonal and/or rhombohedral polytypes:

$16H_{11}$ $tf5tf4(f2f1)_2$ and
$48R_7$ $tf5(t)_2f1f1f2f1$;
$30R_1$ $(t)_2f1f1f5$ and
$48R_6$ $(t)_2f1f1f5tf1f2$;

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$20H_{15}$ *tf2f1tf2f1tf2of1* and
$60R_6$ *f5f1f1tf2f1tf2of1*;
$22H_9$ *f5f1f1f5f1of1f2f2f1f1* and
$66R_6$ *f5f1f1f5f1f1f2f1f2of1* and
$66R_7$ *f5f1f1f5f1f2f1f1f2of1*;
$14H_9$ *tf2f1f2f1f2f1* and
$16H_1$ $(t)_2f2f1(t)_2f2f1$ and
$18H_1$ $(t)_7f2f1$;
$12H_{10}$ *f5tf4f2of1* and
$36R_8$ *f5f4f2of1t*.

On this basis the possible mechanisms for the transitions between different polytypes during the growth of the crystals and/or during solid-state transformations are now being investigated.

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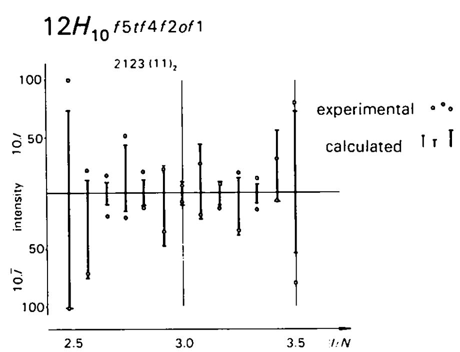

Fig. 1. Diagram of intensities of 10.*l* and 1$\bar{1}$.*l* reflections (+1 and −1) measured experimentally and calculated theoretically for the CdI_2 polytype. Figs. 2–21 show similar diagrams for other polytypes of CdI_2

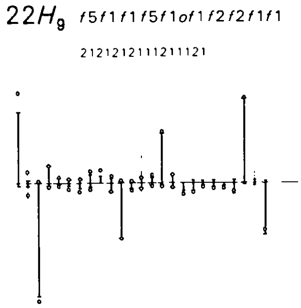

Fig. 4

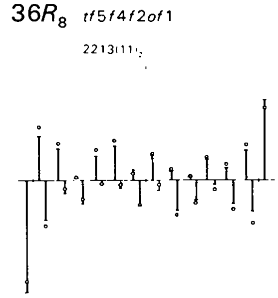

Fig. 5

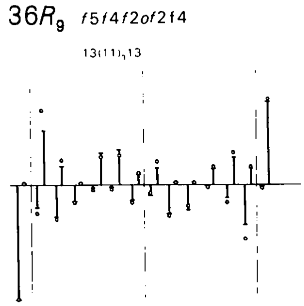

Fig. 6

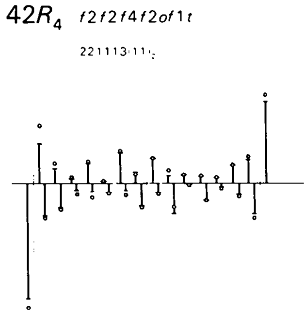

Fig. 7

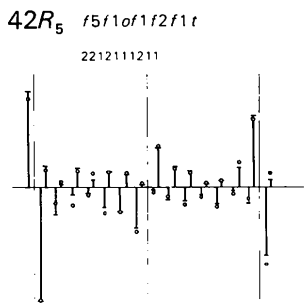

Fig. 8

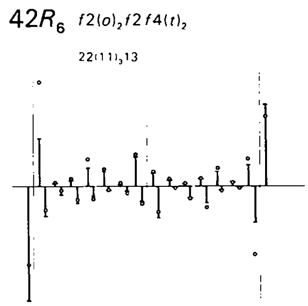

Fig. 9

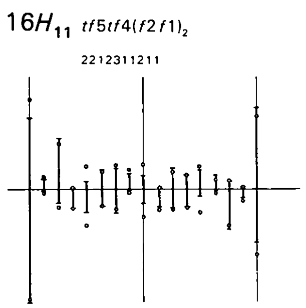

Fig. 2

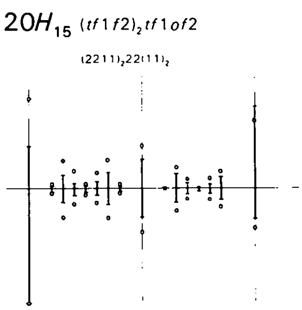

Fig. 3

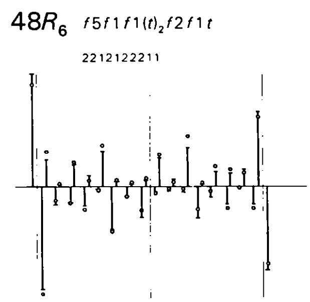

Fig. 10

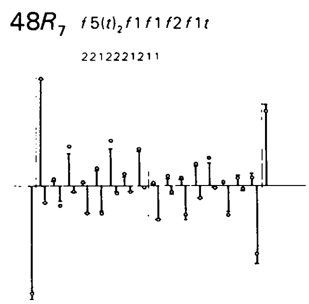

Fig. 11

$54R_8$ $f2f2f1f1(t)_3f2f1$

$211121(22)_2 11$

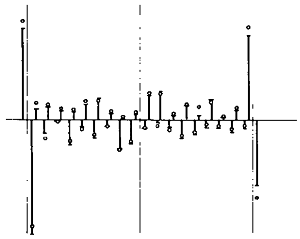

Fig. 12

$60R_4$ $f5f1f1f5f1(o)_4f1$

$2121212(11)_4 1$

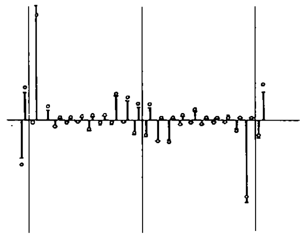

Fig. 13

$66R_6$ $(f5f1f1)_2f2f1f2of1$

$(2121)_2 2112(11)_2$

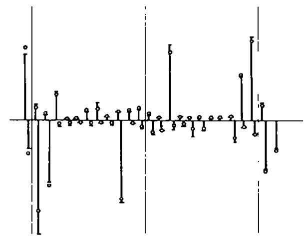

Fig. 18

$66R_7$ $f5f1f1f5f1f2f1f1f2of1$

$212121211212(11)_2$

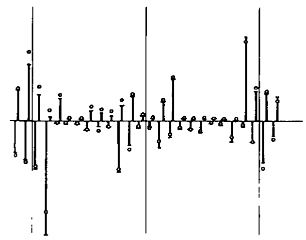

Fig. 19

$60R_5$ $f5f1(o)_2f1f2f1(t)_3$

$(22)_2 12(11)_2 1211$

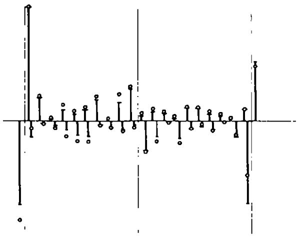

Fig. 14

$60R_6$ $f5f1f1tf2f1tf2of1$

$2121221122(11)_2$

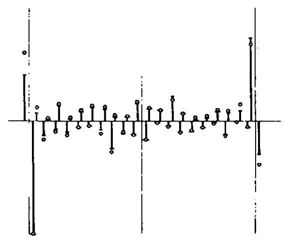

Fig. 15

$84R_6$ $tf2of2f4(t)_4f2(o)_3f1$

$22(11)_2 13(22)_2(11)_4$

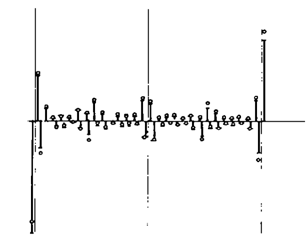

Fig. 20

$108R_2$ $f5f4f5(t)_{11}f4(t)_3$

$222131(22)_5 23$

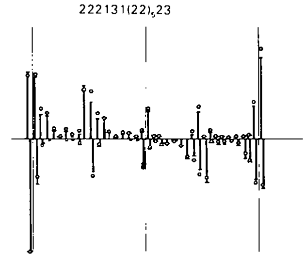

Fig. 21

$66R_4$ $(t)_6f2f2f1of1$

$(22)_3 21112111$

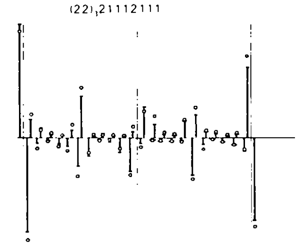

Fig. 16

$66R_5$ $(t)_3f2of2f4f2(o)_2f1$

$(22)_2(11)_2 132(11)_3$

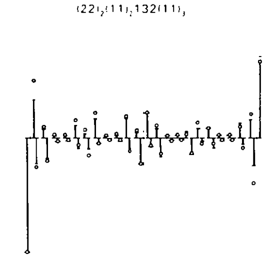

Fig. 17

References

CHADHA, G. K. (1982). *Acta Cryst.* B**38**, 3009–3011.

CHAUDHARY, S. K., CHADHA, G. K. & TRIGUNAYAT, G. C. (1983). *Acta Cryst.* C**39**, 675–677.

GIERLOTKA, S. & PAŁOSZ, B. (1983). VIIth Int. Conf. on Crystal Growth, Stuttgart.

GIERLOTKA, S. & PAŁOSZ, B. (1984). *Acta Cryst.* C**40**, 905–907.

JAIN, P. C. & TRIGUNAYAT, G. C. (1978). *Acta Cryst.* B**34**, 2677–2689.

PAŁOSZ, B. (1982). *Acta Cryst.* B**38**, 3001–3009.

PAŁOSZ, B. (1983*a*). *Phys. Status Solidi A*, **80**, 11–42.

PAŁOSZ, B. (1983*b*). *Acta Cryst.* C**39**, 521–528.

PAŁOSZ, B. (1983*c*). *Acta Cryst.* C**39**, 1160–1163.

PAŁOSZ, B. & GIERLOTKA, S. (1984). *Z. Kristallogr.* **166**, 53–62.

PAŁOSZ, B. & PRZEDMOJSKI, J. (1982*a*). *Cryst. Res. Technol.* **17**, 1513–1521.

PAŁOSZ, B. & PRZEDMOJSKI, J. (1982*b*). *Cryst. Res. Technol.* **17**, 759–765.