Polytype		Space group	Lattice parameters			
R	Z		a[Å]	b[Å]	c[Å]	γ[°]
20	11	Pcab	12.08	13.94	4.53	-
3M	21	$P2_1/b$	20.92	13.94	4.53	120.00
40	22	Pcab	24.15	13.94	4.53	-
4M	31	$P2_1/b$	25.14	13.94	4.53	106.10
$5M_1$	32	$P2_1/b$	31.95	13.94	4.53	109.12
$5M_2$	2111	$P2_1/b$	31.95	13.94	4.53	109.12
$5M_3$	41	$P2_1/b$	30.38	13.94	4.53	96.56
60	33	Pcab	36.22	13.94	4.53	-
$6M_1$	51	$P2_1/b$	38.82	13.94	4.53	111.05
$6M_2$	42	$P2_1/b$	36.88	13.94	4.53	100.87
80	44	Pcab	43.30	13.94	4.53	-

R-Ramsdell notation O-orthorombic
Z-Zdhanow notation M-monoclinic

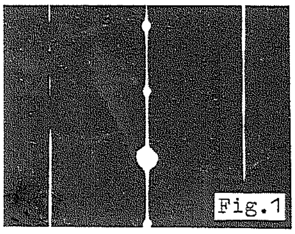


Fig.1

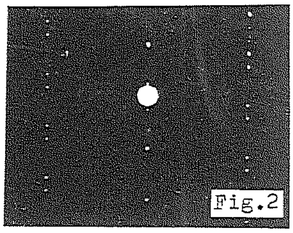


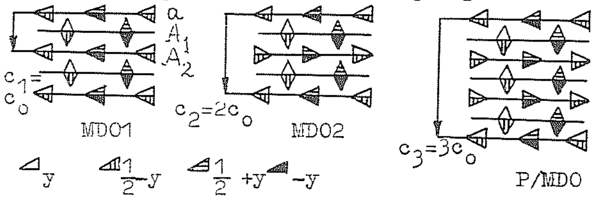
Fig.2

20. 3–3 OD-FAMILY $RAl_3(BO_3)_4$(R=Y,Nd,Gd) AND ITS MDO-POLYTYPES. By E.L.Belokoneva, T.I.Timtschenko, Geological Faculty of the Moscow State University, 117234, Moscow, USSR.

Three structures were found for borates $RAl_3(BO_3)_4$(R=Y,Nd,Gd):one rombohedral and two monoclinic existing at different temperatures. The structures may be considered consisting of two kinds of layers ($A_{1,2}$) wich are parallel to one of the rombohedral plane in the rombohedral structure and parallel to the plane ab in two other monoclinic structures(Belokoneva,Timtschenko,Kristallographiya(1983),28,1118,Zvyagin,Belokoneva,Kristallographiya(1984),29, __) Symbols for OD-groupoid family of category IY (Dornberger-Schiff,Acta Cryst.(1982),A38,483, Dornberger-Schiff,Grell,Acta Cryst.(1982),A38, 491) may be indicated as

A_1	A_2
$[Al_2B_2O_{10}]$	$[RAlB_2O_{10}]$
C12/m(1)	C12(1)
[1 2 (1)]	$[1 \overset{2}{=} (1)]$ $\bar{1}$

Schematic representation of OD-groupoid family



20. 3–2 STUDY OF POLYTYPISM IN GaS USING HREM AND CBED. By T.Bastow, P.Goodman, Whitfield, H.J; Division of Chemical Physics, CSIRO, Australia, and A.Olsen, Physics Department, University of Oslo, Norway.

It has generally been held that a single β-phase with relatively high stacking-fault energy exists for GaS, in contrast to the polytypism of GaSe which arises from alternative stacking sequencing (Basinsky, Z.S., Dove, D. and Mooser, E (1963) J.App.Phys.34,469).

In order to resolve conflicting evidence more recently obtained from several sources (e.g. Zeil, J.P. Meixner, A.E. and Kasper, H.M. (1973) Sol.State Comm.,12,1213), microcrystals of GaS prepared without high-temperature annealing were studied by a combination of CBED and HREM.

As a result a polytype, previously described as a high pressure form (d'Armour, H., Holzapfel, W.B., Polian, A. and Chevy, A. (1982). Sol.State Comm.,44, 853) was identified as a major constituent. This phase, unlike the β-phase , appears to have a relatively low stacking-fault energy. The common Buerger's vector was identified by CBED analysis, while the stacking sequence of the majority component was determined from HREM images.

It was concluded that GaS has (at least) two stable polytypes, which differ from those of GaSe in incorporating relative rotations between the structural layers.

20. 3–4 STRUCTURES OF POLYTYPE CELLS OF CdI_2 AND THEIR FORMATION DURING GROWTH. By S. Gierlotka and B. Pałosz

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It has been suggested that polytypes are multiphase structures intermediate between simple basic structures [Pałosz, B. Phys. Stat. Sol. (a) 80, 11-42 (1983)]. On the basis of this approach some general rules of construction of polytype cells (structural series) have been derived [Pałosz, B. Acta Cryst. B38 3001-3009 (1982)] and next they were succesfully used for identification of tens of polytypes of CdI_2 [e.g. Gierlotka, S. and Pałosz, B. Acta Cryst. (1984) submitted] and SnS_2 [Pałosz, B., Pałosz, W. and Gierlotka, S. Acta Cryst (1984) submitted]. In the present study the structures of more than 200 large period polytypes found in solution grown CdI_2 crystals were analyzed. Several different alcohols were used as solvents. It was found that: (i) about 70% of polytypes grown from n-propyl and isobutyl alcoholic solutions have two-phase 2H-4H structures (structures intermediate between 2H and 4H, see structural series S I and SII; Pałosz, B. Acta Cryst. B38 3001-3009 (1982)] and (ii) 74% of polytypes grown from isoamyl alcohol solutions have one-phase structure $4H_a$-$4H_b$, where $4H_a$ and $4H_b$ represent the same basic structures 4H but oriented differently (c.f. structural series SIII and SIV [Pałosz, B. Phys. Stat. Sol. (a) 80, 11-42 (1983)].

It was established that the frequencies of occurrence of layers o and t (representing here structures 2H and 4H) in a polytype cell are correlated with relative stabilities of basic structures 2H and 4H in given conditions.
It was observed that in some specific conditions pure large polytypes form, in others disordered structures occur frequently. The mechanism of formation of polytype structures in CdI_2 is in case (i) the competition between 2H- and 4H-type stackings of molecular layers and in case (ii) the competition between differently oriented domains of 4H-type stackings (e.g. a slip along [11.0] direction and generation of fault sequences f4f5). The present study do not allow us to decide in which way the inter-phase boundaries created during growth are repeated periodically and form large period polytypes.

20.3–5 SOME ASPECTS OF SYMMETRY OF POLYTYPE STRUCTURES MX_2. By B.Pałosz and S. Gierlotka

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Determination of the symmetry of a polytype may be performed directly on the basis of X-ray pattern, while the determination of the space group is possible only after complete determination of the layer stacking of a polytype cell. The information of a space group of a polytype is practically useless in the analysis of the reasons for polytypism and in the description of the structural behaviour of the crystals. For the characterization of polytype structures we suggest the use of the t-o-f molecular layer notation [Pałosz,B. Z.Krist. (1980) 153, 51-72] where the sequences which form polytypes may be divided into hexagonal- and rhombohedral-type stackings. In this notation it is clearly seen that hexagonal and rhombohedral structures are fully equivalent structures: a hexagonal cell may in some cases be constructed only of rhombohedral-type arrangements of layers of which a rhombohedral cell may also be composed. Similarly, hexagonal-type arrangements of layers may form hexagonal as well as rhombohedral polytypes. The existence of such semi-hexagonal and semi-rhombohedral structures have been confirmed experimentally in a tens of identified polytypes of CdI_2 and SnS_2; Pałosz,B. Acta Cryst. C39 (1983) 1160-1163, Pałosz, B., Pałosz,W. and Gierlotka, S. Acta Cryst. (1984) submitted.

20.3–6 POLYTYPISM, SUBGROUP RELATIONS AND SUPERPOSITION STRUCTURES. By O. Jarchow, Mineralog.-Petrogr. Inst. der Universität Hamburg, Grindelallee 48.

A new method of derivation and description of of polytype structures will be presented.
All space groups of the hexag. and tetragonal system and their subgroups are decomposed in layer groups parallel and perpendicular to the symmetrical directions and arranged to the a,b-plane of layer dimensions. For space groups and their subgroups of the 6mm and 4mm point groups existing only one kind of layer groups in every space group. In all the other space groups their exist two maximum and one minimum layer groups, with the minimum group as commen subgroup in the both max. groups.
All in all we find 409 different sequences with maximum and 212 with a minimum symmetry of the layers.
As known from disordered polytypes, pseudotranslations a/2; a/4;(-a+b)/3 etc. between adjacent layers give rise to sharp and diffuse spots in diffraction images. The sharp spots belong to a superposition structure (SPS) with a regular space group (Dornberger-Schiff,1964), that means, they belong to one of the regular sequences. The transition from SPS to polytypes may be described by transformations like ma, nb, pc, These transformation matrices together with the symmetry of the SPS give the entrance of tables, which allow to determine the different classes of polytypes. From other tables, containing the transformed symmetry operators, we get the informations about space group and partial operators. To avoid a description by partial symmetry operators, we take in account the strong relations between polytypes and their SPS.
Above all the MDO concept of Dornberger-Schiff (Abh. Dt. Akad. Wiss. 1964) about polytypes with maximum degree of order has given new advances in structure determination of polytypes. It will be shown, that these MDOs are in close relationship to twin- and antiphase domains defined by Wondratschek & Jeitschko (Acta Cryst. A 32, 664) and that the use of group-subgroup relations have also many advantages in derivation and description of polytypes.
By generalisation of the procedure in a simple way it is also possible to include polytypes without SPS and also with different kind of layers.
The usefullness and practical application of the method will be demonstrated on some examples.