

where G_1 is generated by a 3_1 screw rotation, C_2 is generated by plane reflections in the side planes of a regular trigonal prisma and hence C_2 is isomorphic to the plane crystallographic group above. Combining these, we get a presentation

$$R3m = (m, s - 1 = m^2 = s^{-3}ms^3m = (s^{-1}msm)^3)$$

belonging to a concave topological polyhedron F . This polyhedron F has only three faces. The face f_m corresponds to the plane reflection $m : f_m \rightarrow f_m$ and the curved faces $f_{s^{-1}}$ are identified by the 3_1 screw-rotation $s : f_{s^{-1}} \rightarrow f_{s^{-1}}$ with screw-rotation angle $\frac{2\pi}{3}$. The presentation is minimal, i.e. F has the minimum number of faces. F is a topological polyhedron, i.e. the body of F is homeomorphic to a 3-dimensional simplex, each face of F to a 2-simplex and so on.

This geometric presentation of the described space groups, illustrated also by Figures, can give a more complete information on the structure of each group.

20.2-8 ON CONSISTENT SETS OF ASYMMETRIC UNITS.

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An asymmetric unit of a space group G is a smallest part of 3-dimensional space from which the entire space may be generated by the action of G . Therefore, all inner points of an asymmetric unit are symmetrically inequivalent to each other with respect to G . Different definitions have been used so far concerning points on the boundaries. Normally, an asymmetric unit is supposed to be simply connected and convex, then it is a polyhedron. These additional conditions can always be fulfilled, because the asymmetric unit may be constructed as Dirichlet domain of a point out of any general point configuration of G . In this case, adjacent asymmetric units share entire faces (the corresponding space tiling is called normal), but the polyhedron may be unnecessarily complicated in shape.

Two sets of asymmetric units have been published, one for all space groups by H. Arnold (in: International Tables for Crystallography, Vol. A (1983), D. Reidel), the other only for cubic ones by E. Koch & W. Fischer (Acta Cryst. (1974), A30, 490). Arnold's set is chosen in such a way, that Fourier summation can be performed conveniently. It contains asymmetric units with non-normal space tilings (cf. e.g. $P4_1$). This is not the case with the Koch-Fischer set which is derived from Dirichlet domains and uses polyhedra with minimal numbers of faces. Both sets do not take care of group-subgroup relations.

For comparative studies (e.g. of relations between crystal structures) sets of asymmetric units would be useful where the asymmetric unit of any space group G is composed of entire asymmetric units of any supergroup $H \supset G$. This, however, seems unachievable because of the complexity of subgroup relations between space groups. Especially for studies of geometrical properties (for a

list of references cf. W. Fischer & E. Koch, Acta Cryst. (1983), A39, 907), however, a less severe restriction is helpful: A set of asymmetric units will be called consistent, if the asymmetric unit of any G is composed of entire asymmetric units of the Euclidean normalizer (Cheshire group) $N_E(G)$. The Euclidean normalizers of space groups belong to 30 types either of space groups or of their degenerations with continuous translations (F.L. Hirshfeld, Acta Cryst. (1968), A24, 301). As a space group occurring as Euclidean normalizer may itself have a Euclidean normalizer of another type, consistent sets of asymmetric units have to be based on a suitable choice for a smaller number of summits ($Im\bar{3}m$, $Ia\bar{3}d$, $P6/mmm$, $P6_222-P6_422$, $R\bar{3}m$, $P4/mmm$, $Pmmm$, $P2/m$, $P\bar{1}$; Z^1_6/mmm , Z^1_4/mmm , Z^1_mmm , Z^1_2/m , Z^2_2/m , Z^3_1).

Outside the cubic crystal system Arnold's set differs from a consistent one only for space groups $P2/m$, $I4_1/a$, $P4_222$, $R\bar{3}$, $P3_112-P3_212$, $R32$ and $R\bar{3}c$. Within the cubic system both published sets are far from being consistent. Summit $Im\bar{3}m$ poses no problems: the unique asymmetric unit of $Pm\bar{3}m$ may be subdivided by a plane containing the twofold axis at $1/2-x$, $1/4$, x . Consistent sets for cubic space groups other than $Ia\bar{3}d$ and its subgroups result if this plane is chosen either at $x+z=1/2$ (case 1) or at $y=1/4$ (case 2). In both cases, the asymmetric units of some space groups may be selected in different ways. Only in case 1 it is possible to restrict to normal space tilings. The number of differently shaped asymmetric units is smaller for case 1 than for case 2. Two other specialized positions of the subdividing plane, i.e. $x-2y+z=0$ (case 3) and $x+y+z=3/4$ (case 4), do not give rise to consistent sets, because the asymmetric units of $Fd\bar{3}m$, $Fd\bar{3}$, and $F4_32$ cannot be made convex. - For $Ia\bar{3}d$ and its subgroups apparently no consistent set of convex asymmetric units can be constructed, but the impossibility of such a set could not be proved so far.

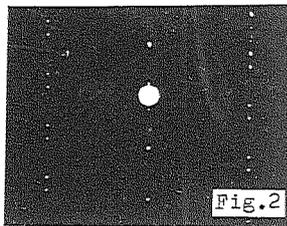
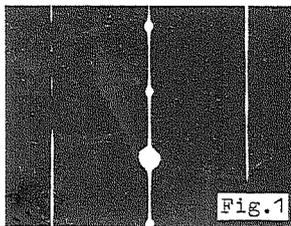
20.3-1 THE POLYTYPES OF THE ORTHORHOMBIC CARBIDE M_7C_3 . By M. Kowalski and W. Dudziński, Institute of Material Science, Technical University of Wrocław, Poland.

The stacking order of the atomic layers in the real crystals of the orthorhombic carbide $/Cr, Fe/_7C_3$ was studied by means of the transmission electron microscopy. The orthorhombic carbides of the type M_7C_3 can be regarded as built up of identical layers of structure stacked parallel to (110) planes. The information about stacking order of the layers is contained in the intensity distribution of diffraction spots observed along $[110]^*$ direction of the reciprocal lattice. In the real crystals regions with completely disordered structure /fig.1/ and ordered sequence of the layers /fig.2/ can be observed. In our earlier paper /XI-th Conference of Material Science, 1983, Częstochowa, Poland/ we described the stacking order using the concept of the polytypism, and we presented the structure of the 20 polytype. Systematical study of the ordered regions in the $/Cr, Fe/_7C_3$ carbides let us determine the structure of the other polytypes. Lattice parameters was determined by analysis of the geometry of distribution of the diffraction spots in the planes $(hk1)^*$ of the reciprocal lattice. The stacking sequence in the unit cell was identified by comparison of the observed intensity distribution of diffraction spots with the intensity calculated for theoretically assumed sequence of the layers. The polytypes found in studied carbides have a following crystallographic dates:

| Polytype | | Space group | Lattice parameters | | | |
|-----------------|------|--------------------|--------------------|-------|-------|-------------|
| R | Z | | a [Å] | b [Å] | c [Å] | β [°] |
| 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 | - |

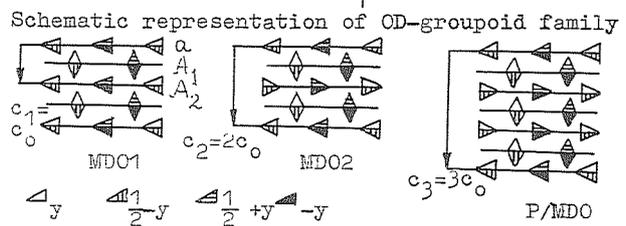
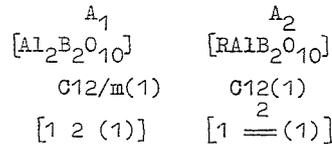
R-Ramsdell notation
Z-Zhdanow notation

O-orthorhombic
M-monoclinic



20.3-3 OD-FAMILY $RA_2(BO_3)_4$ (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 $RA_2(BO_3)_4$ (R=Y, Nd, Gd): one rhombohedral and two monoclinic existing at different temperatures. The structures may be considered consisting of two kinds of layers (A_1, A_2) which are parallel to one of the rhombohedral plane in the rhombohedral structure and parallel to the plane ab in two other monoclinic structures (Belokoneva, Timtschenko, Kristallografiya (1983), 28, 1118; Zvyagin, Belokoneva, Kristallografiya (1984), 29, 1118). Symbols for OD-groupoid family of category IV (Dornberger-Schiff, Acta Cryst. (1982), A38, 483; Dornberger-Schiff, Grell, Acta Cryst. (1982), A38, 491) may be indicated as



20.3-2 STUDY OF POLYTYPISM IN GaS USING HREM AND CBED. By T. Bastow, F. 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 δ -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., Holzappel, W. E., Polian, A. and Chevy, A. (1982) Sol. State Comm., 44, 853) was identified as a major constituent. This phase, unlike the δ -phase, appears to have a relatively low stacking-fault energy. The common Burger'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 POLYTYPIC 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 successfully 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-4H₁, where 4H and 4H₁ 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)]).