20.2–5 PERMISSIBLE INDICES FOR MAXIMAL ISOMORPHIC SUBGROUPS OF 2-DIMENSIONAL SPACE GROUPS. Y. Billiet, Faculté des Sciences et Techniques, Université de Bretagne Occidentale, 6, avenue Le Gorgeu, 29283 Brest, France, et Recherches en Symétrie Cristallographique à Sétif, A5, 35, Cité du 8 mai 1945, Sétif, Algérie.

In dimensions 2 and 3, maximal "translationengleich" subgroups and maximal non-isomorphic "klassengleich" subgroups always are finite in number. On the contrary, there exist maximal isomorphic subgroups always in infinite number for any 2- or 3-dimensional space group. However the permissible values for the index are limited. As an example, here are given the suitable values for 2-dimensional maximal isomorphic subgroups.

p1, p2, pm, pg, p2mm, p2mg: any prime integer.
cm, p2gg, c2mm: any odd prime integer.

p4: 1/ any prime integer of the type $k_1^2+k_2^2 \neq 4k_3+1$;

2/ any integer of the type $k_1^2+k_2^2 = (4k_3+3)^2$ where $4k_3+3$ is a prime integer.

p4mm: 1/ the number 2; 2/ any integer of the type k^2 where k is a prime integer.

p4gm: any integer of the type $(2k+1)^2$ where 2k+1 is a prime integer.

p3, p6: 1/ any prime integer of the type $k_1^2+k_2^2-k_1k_2$;

2/ any integer of the type $k_1^2+k_2^2-k_1k_2 = (3k_3+2)^2$ where $3k_3+2$ is a prime integer.

p3m1, p31m: any integer of the type k^2 where k is a prime integer.

p6mm: 1/ the number 3; 2/ any integer of the type k^2 where k is a prime integer.

20.2–6 ON SUBGROUPS OF SPACE GROUPS. P. Engel, Laboratory for crystallography, Freiestrasse 3, CH-3012 Berne, Switzerland.

Group-subgroup relations are of interest in several fields in crystallography. Tables of maximal subgroups of space groups are contained in the International Tables, Vol. A (D. Reidel publishing company, Dordrecht, 1983). Using these Tables however, a systematic determination of all subgroups of a space group proves to be very tedious. A novel computer program has been developed which allows a systematic determination of all subgroups of the space groups. For a space group G with given arithmetic crystal subclass and given sublattice the program calculates all possible subgroups H following an algorithm proposed by Senechal (Acta Cryst. A36 (1980) 845-850). Subgroups which are conjugate under G or alternatively under the Euclidean normalizer $N_E(G)$ are eliminated. For each Bravais class the transformation laws for the generation of all possible sublattices are derived. The space-group type of a subgroup is determined using a procedure which takes into account only geometric properties of the subgroup which remain invariant under affine transformations.

The subgroups of a space group G are classified according to their space-group type. Subgroups belonging to the same space-group type are arranged in series, each serie containing an infinite number of subgroups. It will be shown that for any space group only a finite number of series of subgroups exists. Examples will be presented.

Among the subgroups the normal subgroups are of special interest. Every normal subgroup determines the kernel of a possible homomorphism. The normal subgroups for all 2- and 3-dimensional space-group types have been determined.

Example: The normal subgroups of space-group type No. 92 $P4_12_12$ (equivalence under $N_E(G)$; $d \geq 0$; $a,c \geq 1$; the index is given in brackets).

sublattice	normal subgroups
1,0,0/0,1,0/0,0,1	$P2_12_12_1(2)$, $C222_1(2)$
1,0,0/0,1,0/0,0,2d+1	$P2_1(8d+4)$
1,0,0/0,1,0/0,0,4d+1	$P4_1(8d+2)$
1,0,0/0,1,0/0,0,4d+3	$P4_3(8d+6)$
1,1,0/-1,1,0/0,0,1	$P222_1(4)$, $P2_12_12_1(4)$
1,1,0/-1,1,0/0,0,2d+1	$2 \cdot P2_1(16d+8)$
a,0,0/0,a,0/0,0,c	$P1(8a^2c)$
2a,0,0/0,2a,0/a,a,c	$P1(32a^2c)$
a,a,0/-a,a,0/0,0,c	$P1(16a^2c)$
a,a,0/-a,a,0/0,a,c	$P1(16a^2c)$
a,0,0/0,a,0	p1(∞)
a,a,0/-a,a,0	p1(∞)
0,0,c	p1(∞)

20.2–7 PRESENTATION OF CRYSTALLOGRAPHIC GROUPS BY FUNDAMENTAL POLYHEDRA. By E. Molnár, Eötvös Loránd University, Budapest, Hungary.

There is a Poincare's method to present a discrete isometry group G by means of a fundamental polyhedron F endowed with a face identification. The identifying isometries generate the group G. The cycle relations, belonging to the edge equivalence classes of F, together with the eventual reflection relations give us the mentioned presentation of G. The author's intention, to give a so-called minimal geometric presentation for each space group, has been realized in most cases, sometimes only by concave topological polyhedra (Molnár, Beiträge zur Algebra und Geometrie (1983) 14, 33). We shall determine these polyhedra presenting minimally those 38 space groups which have semi-direct decomposition $G = G_1 \circ C_2$, where C_2 is an invariant Coxeter subgroup generated by plane reflections and G_1 is a so-called rod group leaving a straight line invariant (e.g. Koch and Fischer, Z.Kristallogr.(1978) 147, 21).

As a typical example let us consider the space group $G = R3m$. Then $G_1 = P3_1(11)$, $C_2 \cong p3m1$, 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 $m : f_m \to f_m$ and the curved faces $f_{s^{-1}}$ f_s are identified by the 3_1 screw-rotation $s : f_{s^{-1}} \to f_s$ 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.

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 occuring 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^16/mmm, Z^14/mmm, Z^1mmm, Z^12/m, Z^22/m, $Z^3\bar{1}$).

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 $F4_132$ 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.

20.2–8 ON CONSISTENT SETS OF ASYMMETRIC UNITS.

By W. Fischer, Institut für Mineralogie, Philipps-Universtät, 3550 Marburg, FRG

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

20.3–1 THE POLYTYPES OF THE ORTHOROMBIC 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 orthorombic carbide $/Cr,Fe/_7C_3$ was studed by means of the transmission electron microscopy. The orthorombic 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 completly 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 analisys 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 comparision of the observed intensity distribution of diffraction spots with the intensity calculated for theoritically assumed sequence of the layers. The polytypes found in studed carbides have a following crystalogaphic dates: