20. SYMMETRY AND THE CLASSIFICATION OF STRUCTURES

20.X-5 QUASICRYSTALINE AND RELATED CRYSTALLINE STRUCTURES. By K.S. Kim. Beijing Laboratory of Electron Microscopy, Chinese Academy of Sciences, P.O. Box 2724, Beijing, P.R. China.

The formation and structure of both the icosahedral and decagonal quasicrystals are shown to be closely related to the structure of the crystalline phase I. A number of icosahedral quasicrystals have been found in Ti-Ni, Ti-Fe, V-Ni-51 and H-M-Ni-51 systems and the equilibrium phases in these systems all contain more than 50% icosahedra in their crystalline structures. Moreover, the orientation relationship between the icosahedral phase and the respective crystalline phase is determined by the orientation of the icosahedra in them. II. The transformation of the Al-Cr icosahedral phase (a25) to Al64Cr2 (2/m) has been analyzed from the group-subgroup point of view. Fivefold and threefold twins were found around the [101] and [145] directions respectively which in turn are parallel to the 3 and 5 axes, respectively, of the icosahedral phase. In other words, the icosahedron serves as the bridge between the structure of the icosahedral phase at one end and the crystalline phase at the other. III. The structures of the decagonal quasicrystal of Al1-M (M=Cr, Fe, Co, Ni, Ru, Rh, Pd) have been studied by XRD and it was shown that the one-dimensional periodicity of this 2D quasicrystal is closely related to one of the unitcell dimensions of the crystalline phase.

20.X-6 ON THE HERMANN-MAUGUIN SYMBOLS. By H. Wondratschek, Institut für Kristallographie, Universität (TH), Karlsruhe, Federal Republic of Germany.

Several proposals for the use of other space-group symbols than those of Schoenflies have been published. One of them is the 'Hermann-Maugin' or 'International' symbolism. The Schoenflies symbols are essentially symbols for the group and do not distinguish the different space-group types belonging to that point-group type. The Hermann-Maugin symbols are genuine space-group symbols (from which the corresponding point-group symbols may be derived by a simple procedure). The constituents of each Hermann-Maugin symbol represent a set of generators of the space group. In the selection of generators, (glide) reflections are preferred to (screw) rotations. Rotoinversions and inversions are used only if unavoidable. This choice together with an appropriate nomenclature make possible to do without the relative positions of the geometric symmetry elements in most cases. From the short (Hermann-Maugin symbol the 'general positions' of the space-group type can be calculated easily. The structure of the symbols allows, moreover, the complete derivation of all space-group types, provided the 32 crystal classes and the 14 Bravais types of lattices are supposed to be known.


The definitions of scientific concepts change with time, reflecting the current state of knowledge. This is as is should be. Crystal symmetry became popular when Hauy (1800) stated his law of symmetry (similar edges, and apices, of the crystal polyhedron are similarly truncated); the truncations were rational faces of a new form, visualized as a whole and represented by the Hauy-Lévy form symbol. --Weiss (1816) and Mohs (1813) introduced analytic geometry in crystallography (origin 0 anywhere inside the crystal) and devised a face symbol (the Weiss coefficients, precursors and reciprocals of the Miller indices). --Bravais (1849) re-enumerated the 32 crystal classes (Hauy (1830), whose paper was to remain unread until Schöncke discovered it in 1891), but his main achievement is his work on lattices (translation groups): 7 point symmetries in lattices, whence the 7 Bravais systems; 14 lattice modes. Whereas Weiss and Mohs were justified in distinguishing hexagonal from trigonal on the basis of the order of the principal axis, observed on the morphology, Bravais was able to discriminate between lattices, hexagonal and rhombohedral, not only theoretically but also empirically (law of Bravais). Bravais' space consists in an infinite set of points (nodes); one of them is taken as 0. New definitions of elements of symmetry use lattice language: an axis is a row line, a mirror is a net plane. --Jordan's paper (1867) ushered in group theory for crystallographers. The group elements are the symmetry operations; the whole group is the symmetry element. By using screw axes, Schöncke (1879) found 16 (one too many) space groups of motions; by adding the glide planes Schöncke (1891) and Fedorov (1891), it was shown by Barlow (1894), found the remaining 165 space groups. --Various generalizations of symmetry (antisymmetry or black-white, color symmetry, etc) were made in the twentieth century, introducing new elements and operations.


The committee has been set up in 1980 to 'consider nomenclature problems concerning symmetry operations and symmetry elements in space groups'. Such problems are known to occur in particular for glide planes:

1. A plane like xy0 is both an a- and a b-gliding plane. The symbol "a" is awkwardly biased.
2. In Cmmm, again two symmetry operations share a plane. One is a reflection (x, y, z), the other (1/2-x, 1/2+y, z) an n-glide reflection. So here xy0 is a mirror plane as well as a n-gliding plane.
3. There are also glide planes for which there is no conventional symbol at all. Corresponding glide reflections are labelled 'g' in I.T. (Intern. Tables for Crystallography, 1983, Vol.A. Dordrecht: Reidel). They occur e.g. in space groups nos. 100, 125, 134, 160 and 225.

It can be concluded that the definition of glide planes by the enumeration in Table 1.3 of I.T. is unsatisfactory. Before proposing new symbols, we require an answer to the question: what is a glide plane? This leads to the question: what is a symmetry element? For which there is no generally accepted answer either. The committee agrees that 'symmetry element' has a much wider meaning than 'symmetry operation'. An explicit concept proposal is at present being discussed. If accepted, it will allow further proposals on symbols to be designed in the near future.