TOPICS

This year, crystallographers may celebrate at least three anniversaries. One of them is so well known that it is hardly necessary to draw crystallographers' attention to it: it is the seventy-fifth anniversary of the first X-ray photographs taken by M. von Laue, W. Friedrich and P. Knipping. With these photographs a new chapter in the history of crystallography has been started. Another anniversary is also related to X-ray investigations: in 1937 M. Renninger described the effect of "Umweg-anregung", also called "Renninger effect", which has become important for theoretical and practical applications of X-ray crystallography.

The third anniversary is twofold. The centenary of the day, when the great Russian crystallographer A. V. Shubnikov was born, has been celebrated with an International Seminar on Symmetry at the Institute for Crystallography of the Russian Academy of Sciences in Moscow in April 1987. The other event that could be celebrated is the centenary of the first and correct formulation of what a crystal structure might be. This formulation was published by F. Haag in 1887 but the publication seems to have been completely forgotten. Nevertheless, this discovery has influenced strongly the way crystallography has developed over the last 100 years.

Crystals are peculiar objects in our natural surroundings. They have certainly been found, stared at and admired since the beginning of mankind. The most striking appearance is the symmetric polyhedral shape which they may exhibit. Oddly enough there seem to be no considerations known which deal with this phenomenon until the late middle ages. Only during the last centuries, ideas on the structure of crystalline matter have been proposed in order to explain and understand rather different aspects of crystals.

A reasonable early assumption considered crystals to be built up of blocks or "atoms" of such polyhedral shapes. An approach of this kind suggested itself even more so when the physical property of cleavage pointed to that building principle. The apparent contradiction for several substances between external shape and cleavage planes could be solved by Haüy in an elegant way about 200 years ago.

Following this period it was rather the physical properties than the shape of crystals whose explanation by the crystal structure awoke the interest of scientists. The mechanical and optical behaviour of crystalline matter had been studied and the results waited for an interpretation on the basis of the arrangement of the particles constituting the crystal and of the forces acting between them. The theories of that time had one feature in common: the parallel arrangement of points, particles, molecules, etc. was assumed to be characteristic for a crystal. Parallel arrangement i.e. periodicity or translational equivalence was considered to be the essential property. Simultaneously, the symmetry of the crystals and its classification drew the attention of scientists: the crystal systems, crystal classes and symmetry types of lattices (Bravais lattices) were derived.

Symmetry, however, caused a difficulty. The point groups, i.e. the symmetries of the external shape and of the macroscopic physical properties had been determined for numerous crystals. The observed symmetries deviated from those of the lattices in many cases. This deviation could be explained only by the assumption that the building blocks constituting the crystal in parallel arrangement had certain symmetry for themselves. Then the symmetry of the crystal was the result of the interplay between the holohedral symmetry of the lattice and the lower symmetry of the "molecule".

A step forward to the solution of this unsatisfactory situation was the introduction of the "regular systems of points" (regelmässige Punktsysteme) by L. Sohncke, following a suggestion of Chr. Wiener. A regular system of points (or of atoms, molecules, etc.) is a periodic arrangement of the constituents where each constituent is surrounded by all the others in exactly the same way.

The constituents, however, need not all be parallel, as had been assumed up to then; they may be obtained one from another also by other operations, as rotations or screw rotations. The essential new point of view was to replace "translational equivalence" by the more general "symmetrical equivalence". According to Sohncke, a crystal was supposed to be an arrangement of particles which could be represented by a regular system of points.

In Sohncke's conception only translations, rotations and screw rotations were possible symmetry operations of a crystal. However, in nature crystals exist which exhibit the symmetries of reflections, inversions and rotoinversions. L. Wulff, who did not follow Sohncke's idea, compared such crystal symmetries with, the possible symmetries of regular systems of points. He found that the symmetries of the well-known minerals dioptase and phenakite could not be explained by any regular system of points. Wulff published this result together with other criticisms. Sohncke rejected all of them with one exception: he could not refute Wulff's symmetry argument just mentioned. Thus, he had to admit that his theory needed some generalization.

This was in 1888. However, already one year before F. Haag had given this generalization in an article "Die regulären Krystallkörper", published in the "Programm des Königlichen Gymnasiums in Rottweil zum Schlusse des Schuljahres 1886-87". In this paper he stated "...Krystalle sind regelmässige Punktsysteme und Combinationen von soichen . . ." (crystals are regular systems of points and combinations of such systems).

Without doubt, such an important statement could hardly be published in a more remote journal. However, at that time the Zeitschrift für Kristallo-graphie und Mineralogie, the only journal devoted in the first line to crystallography, supplied its issuewith outstanding review sections. In these sections, important crystallographic papers were cited from other sources and reviewed by prominent crystallographers. Haag's paper was made known by E. Blasius in Vol. 14 (1888) 501-502. Blasius described the contents, mentioned some results and formulae he found to be of more mathematical interest and continued: 'On the other hand, the ideas of the author are of great importance for the theory of crystal structures. . . . '. He then quoted the main result word for word. Thus, Haag's paper with its hidden central statement was brought to the knowledge of crystallographers.

Nowadays, Haag's definition is the background for most data by which crystal structures are described: one representative point (centre of an atom) of each regular system of points is given by its coordinates. The other atoms are then generated by the symmetry operations of the space group of the crystal structure.

X-ray crystallography could not have been developed so rapidly if the theory of space groups and crystal structures had not been available when X-ray investigations began in 1912. The stirring idea of Friedrich Haag as well as the pioneering work of L. Sohncke, L. Wulff, E. S. Fedorov, A. M. Schoenflies, W. Barlow and others had started a new phase in the studies which had occupied the minds of many crystallographers during the last 300 years. It was the grounding on which the edifice of X-ray crystal structure determination could be successfully founded and erected to its present imposing but still growing greatness.

Nowadays, determination of crystal structures is routine work for many substances and giant structures like proteins, starch etc. are tackled with greater and greater success. Furthermore, X-ray crystallography is transgressing its traditional borders of three-dimensional periodic structures. Super-structures are being solved successfully and non-periodic structures, e.g. incommensurate phases or quasicrystals, are accessible by the development of more powerful X-ray equipment and generalized crystallography. Thus, the combination of experiment and theory opens new prospects for our knowledge.

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