19.2–5 INTERACTIVE GRAPHICS PROGRAMS INVOLVED IN THE INTERPRETATION OF DIFFRACTION DATA.

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Procedures and exercises developed for use in crystallographic courses intended to be integrated in various disciplines such as physics, chemistry, geology and engineering (I.U.Cr. Abstract 24.1-1, 1975) have now been reorganised to make use of computer simulations of films and stereographic projections. The simulations can be generated interactively by the student using a graphics terminal. When suitable solutions to problems have been arrived at using the terminal, final hardcopy can be obtained on either a pen plotter or an electrostatic plotter.

Available programs can simulate Laue, powder, rotation, oscillation and Weissenberg films as well as being able to produce stereographic projections and various types of nets. Such patterns were used as illustrations in a previous poster (I.U.Cr. Abstract 19.4-03, 1981).

The resemblance between diffraction patterns and real films can be increased by enhancing particular reflections in various ways. In the case of the Laue pattern this is done for reflections produced by the characteristic radiation, whereas on a rotation or oscillation pattern enhancement is used to indicate the multiplicity.

The relation between the symmetry of the crystal structure and the diffraction pattern can be shown by using an interactive molecular graphics package such as RAL PLUTO78, which has also been adapted to display framework structures using the type of polyhedra which are familiar to mineralogists.

Video recordings of real-time operation can be made for use in lectures. It is intended that such a video recording will accompany this poster.

19.2–6 COORDINATION OF VOIDS. By G. Ruban,

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The determination of effective coordination numbers (Hoppe, 1970) by the method of central projections (Ruban, 1984) is not affected by any voids occurring in the structure. However due to crystal symmetry and radii selected there is a correlation between particles and voids. The neighbourhood of voids (channels, cages) has been investigated, results are represented for the basic lattice types of crystal chemistry and for some more complicated cases, e.g. zeolithes, clathrates, cyclodextrines.

Literature:

Hoppe, W. "The Coordination Number - an Inorganic Chameleon", Angew. Chem. Int. Ed. 9 (1970) 25-34

Ruban, G. "The Aspects of Adjunction and Coordination in Mineralogy" Fortschritte der Mineralogie 62 (1984) in press.

19.2–7 PATTERNED POLYHEDRA - A TEACHING AID TO ILLUSTRATE GROUP-SUBGROUP RELATIONSHIPS. By W. Fischer,

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Cubes of pyrite crystals reveal their true point-group symmetry $m\bar{3}$ - instead of $m\bar{3}m$ of the sheer polyhedra - by striation of the faces. This principle may be generalized as follows: The faces of a polyhedron with symmetry G are supplied with striae or similar patterns such that the patterned polyhedron shows the symmetry of a subgroup $U \subset G$.

In this way a set of wooden models has been prepared that illustrates the relationships from $m\bar{3}m$, 6/mmm, 4/mmm, mmm, 2/m, and $\bar{1}$ to the other point groups of the corresponding crystal family. The polyhedra are shaped like the corresponding unit cells, except for the hexagonal family where hexagonal prisms are used. The symmetry of each face is indicated, symmetrically inequivalent faces being differently patterned. With two exceptions simple striation is used: (1) A 3-, 4- or 6-fold rotation axis perpendicular to the face requires simultaneous striation in two or three directions. (2) In absence of a 2-fold rotation axis perpendicular to the face, direction and counter-direction have to be distinguished; this is achieved by wedge-shaped patterns. Point groups $\bar{6}2m$, $\bar{3}m$, 3m, 32, and $\bar{4}2m$ are represented in both orientations with respect to the conventional unit cell. Each polyhedron of the set shows as much symmetry information as possible on each of its faces.

In contrast, a modification of this concept may use a minimum of striation; the symmetry of a cube, e.g., is reduced to 1 if two adjacent faces are independently striated in general directions.

19.2–8 A DEMONSTRATION OF TEACHING CRYSTAL GROWTH: GROWTH OF LOW-MELTING ORGANIC CRYSTALS FROM UNDERCOOLED MELT AND BY THE CZOCHRALSKI TECHNIQUE: By Th. Scheffen-Lauenroth, R.A. Becker and H. Klapper,

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Growth from undercooled melt: Melts of organic materials can be strongly undercooled without inducing spontaneous nucleation. If a seed crystal is placed into a somewhat undercooled melt, it can grow in 10-40 hours, depending on the degree of undercooling, to a highly perfect crystal of a few cm diameter. Since organic crystals have, in general, a high α-factor ($\alpha \cong 6$ for benzophenone), growth takes place on habit faces. Thus, organic crystals grown from undercooled melt are completely surrounded by plane growth faces.

A simple growth chamber with benzophenone crystals (freezing temperature ≅48°C) growing from undercooled melt is shown in action. One growth run will take 1-1.5 days and will then be repeated. When starting a new growth run, the procedure of optimal seeding-in is demonstrated.

Czochralski growth: A simple Czochralski apparatus growing crystals of benzophenone or salol (freezing point ≅42°C) is shown in action. It consists of a temperature-controlled chamber with circulating air, in which a double-walled glass vessel containing the melt is placed. The vessel with the melt is heated up by hot water from a bath thermostat to a temperature some degrees above the melting point. The crystal is cooled by the circulating air, the temperature of which is adjusted to 5 - 15°C below the melting point.

In addition, the growth procedures are schematically shown and explained with the aid of a colour computer-graphic video presentation. This performance includes explanations of the growth chambers, the seeding-in procedures, etc.. A collection of benzophenone and salol crystals grown by both methods will be exhibited.