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Symmetry of STRUCTURE

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Abstracts

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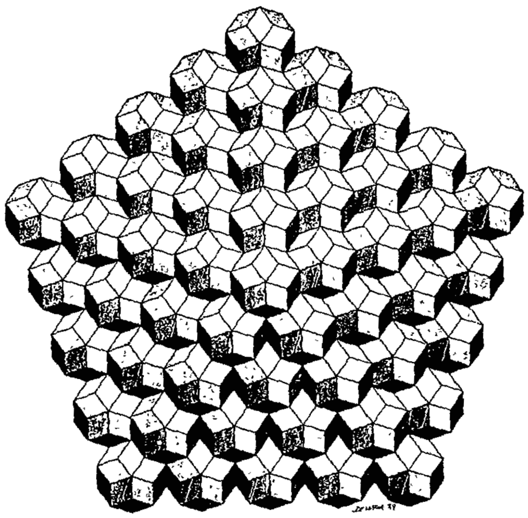

Edited by Gy. Darvas and D. Nagy

Buda pest

August 13-19, 1989

hungary

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CORRELATION BETWEEN CRYSTAL SYMMETRY AND SYMMETRY OF THE FINE STRUCTURE OF ELECTRON DIFFRACTION PATTERNS

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The various electron diffraction techniques are most versatile and reliable methods for the determination of the symmetry of crystalline samples. Both the point group and the space group of crystals may be determined by means of convergent-beam microdiffraction. Furthermore, the symmetry of the diperiodic crystal surfaces can be deduced from low-energy electron diffraction (LEED) as well as reflection high-energy electron diffraction (RHEED) patterns. Besides the structural symmetry obtained by analysing the geometry and the intensities of the patterns the interpretation of the shape of the reflections may reveal the symmetry of the external form of the crystals. Within the kinematical theory of diffraction, the mutual connection between the diffraction pattern and the reciprocal lattice is elucidated by the EWALD sphere construction. As the reciprocal lattice is the Fourier transform of the crystal lattice (see fig. 1), both the position and the shape of the diffraction spots are specified by the Fourier transform of the distribution of scattering objects in the crystal. The position of the diffraction spots is determined by the internal structure of the crystal, but the shape of the diffraction spots is mainly determined by the external form of the crystal as well as by the presence of crystal defects. The influence of the external form of the finite lattice on the shape of the diffraction spots is illustrated in fig. 2.

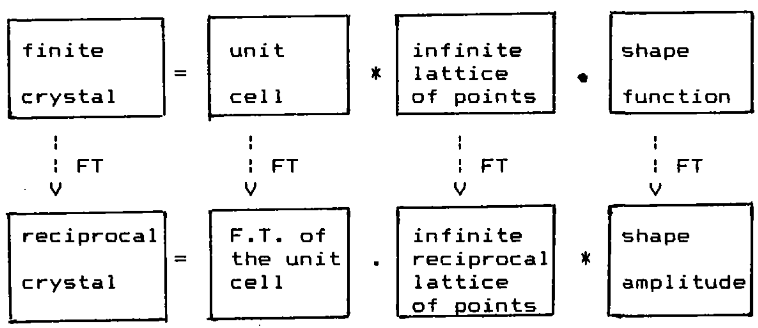

Fig.1: Scheme of the Fourier transform of a finite crystal (• multiplication, * convolution)

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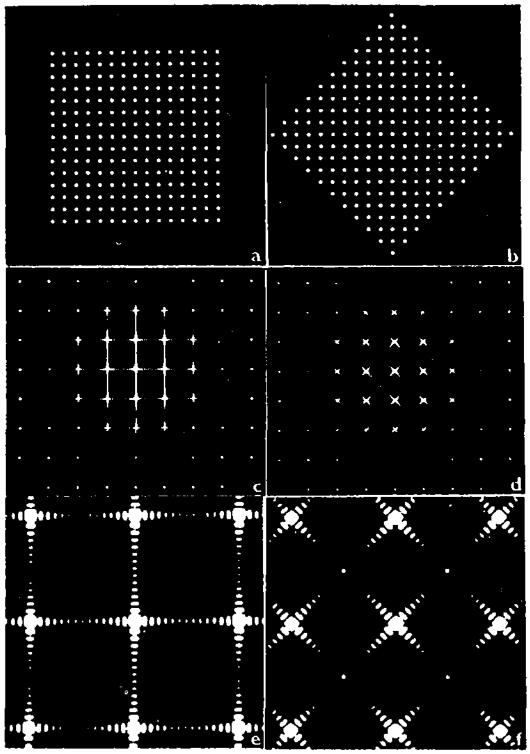

(a), (b)- two-dimensional lattices of the same structure but with different external boundaries

(c)-(f)- Fraunhofer diffraction patterns from (a),(b) obtained by optical diffractometry

(c), (d)- the whole central region of the patterns

(e), (f)- a detail showing the shape of the diffraction spots

Fig. 2: The influence of the shape transform

In transmission electron diffraction of small crystals spots are frequently observed which have distinct fine structure consisting of streaks, satellites or elongations. This fine structure is determined by the intersection of the EWALD sphere with the three-dimensional intensity distribution of the diffracted beams. The contribution of the crystal shape to the shape of the diffraction spots can be theoretically described by the crystal shape amplitude $S(\vec{p})$ which in fact is the Fourier transform of the shape function $s(\vec{\xi})$ of the crystal. The shape of the diffraction spots may be related to a single shape amplitude only if the lattice is sufficently large, i.e. if it is formed by a large number of unit cells (more than 30) in any direction. This is usually the case in crystallographic applications. If this condition is not fulfilled, the shape of the diffraction spots should be related to the so called lattice amplitude, which is a periodic function expressable as a superposition of the shape amplitudes. The concept of the shape amplitude was introduced by von Laue (1936). General algebraic expressions were derived (Komrska, 1988), which enable numerical evaluation of the shape amplitude of any crystal polyhedron. The derivation is based on the repeated Abbe transform, which makes it possible to express algebraically the multiple integrals defining the shape amplitude. The shape amplitude is a special case of the Fourier transform of a real function. Hence, the algebraic expressions must possess all the properties that follows from this fact.

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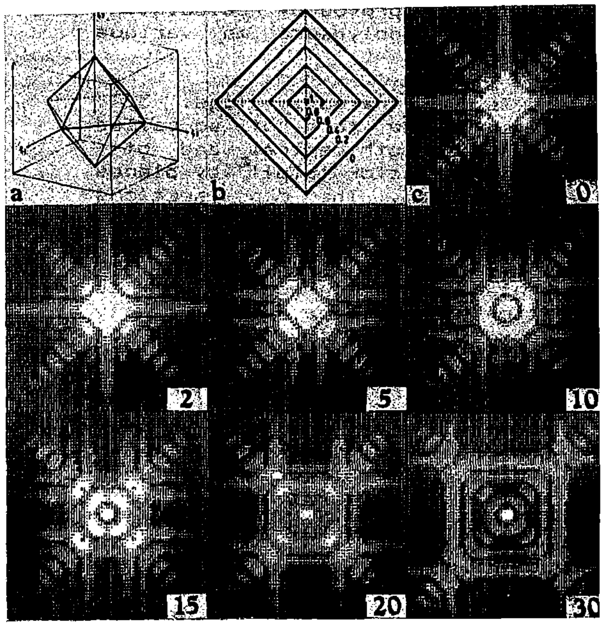

Fig.3: Crystal shape factor map for an octahedron in (001)-orientation;
(a)-orientation relationship of octahedron in circumscribed cube,
(b)-thickness isolines
(c)-cross-sections of shape factors $|S|^2$,

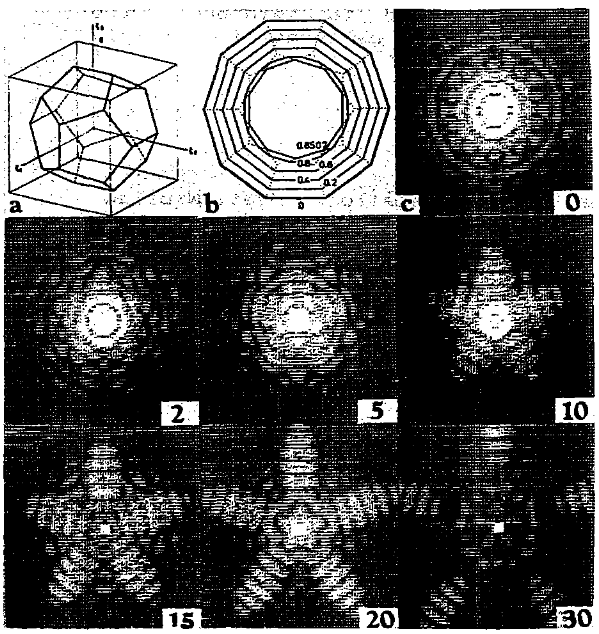

Fig.4: crystal shape factor map for a regular pentagonal dodecahedron in ($0\ \tau\ 1$)-orientation relationship of pentagonal dodecahedron in circumscribed cube,

(b)-thickness isolines

(c)-cross sections of shape factors $|S|^2$

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The main properties are:
The shape amplitude S($\vec{p}$) has all the symmetry elements of the shape function s($\vec{\xi}$) of the crystal.
The shape amplitude of a crystal with centrosymmetric shape is always a real function.
The properties of the shape amplitude were proved by calculating the shape amplitudes of the Platonian polyhedra in various orientations (Komrska, Neumann, 1986).

The computer simulation procedure is illustrated in figs. 3,4. The numerical results are presented in the form of so-called crystal shape factor maps representing both central and off-central cross-sections through the shape factor $|S(p)|^2$ by planes perpendicular to the incident electron beam. The cross-sections of the shape factor for a regular pentagonal dodecahedron in ($0\tau1$)-orientation, *i.e.* *parallel* to a five-fold axis (fig. 4) might be useful for interpretation of diffraction patterns of small quasi-crystals, were a pentagonal dodecahedral shape is possible. The central cross-section of the shape factor clearly shows the tenfold symmetry corresponding to the fivefold axis of s($\vec{\xi}$). The off-centre cross-sections obviously exhibit the loss of the centrosymmetry which leads to the fivefold symmetrical cross-section.
The computer simulation of the crystal shape factor was *applied* to the interpretation of the shape and symmetry of transmission electron diffraction reflections from small polyhedral gold and palladium crystals having octahedral and tetrahedral habits (Neumann et. al., 1988). The fine structure of the experimental diffraction spots may be compared with that of simulated spots obtained from the two-dimensional intensity distribution at plane intersections with the corresponding shape amplitudes. The different off-centre cross-sections can be assigned to the corresponding components of the actual deviation parameter of a diffraction spot from the Ewald sphere for any given size of the crystal. *The method can also be used to interpret* the differences in the symmetry of diffraction patterns of multiply twinned particles and quasi-crystals.

References

Komrska,J.(1988) Optik 80,171-183
Komrska,J.,Neumann,W.(1986) Tenth Eur.Crystallogr. Meet.,Wroclaw Poland.Abstracts 450-451
Laue,M.v.(1936) Ann. Phys. (Leipzig) 26,55-68
Neumann,W. et al.(1988) Acta Cryst. A44, 890-897