

17.01 - Symmetry of Crystals and Quasicrystals

MS-17.01.01 SEMI-INVARIANT DESCRIPTION OF THE POINT GROUP SYMMETRIES BY HIGH-ORDER MOMENTS
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The spatial distribution of a three-dimensional function can be characterised by calculating all the three-dimensional moments $\mu(p,q,r)$ of order k , $k = 0, 1, 2, 3, \dots$ and p, q, r running over all non-negative integer values so that $p+q+r=k$. (M.G. Kendall and A. Stuart, *The Advanced Theory of Statistics*, Charles Griffin and Co., 1969, Vol.1, Chap. 3-4). The moments are k -rank tensors and they have either covariant or contravariant character according to the type of coordinates used for their computation (L.A. Patterson, *International Tables for X-ray Crystallography*, Kinoch Press, 1972, Vol. 2, Chap. 2).

The symmetry properties of the function influence the values of the moments reducing the maximum number, $(k+1)(k+2)/2$, of independent components of each moment, as well as establishing relationships among them (J. N. Nye, *Physical Properties of Crystals*, Oxford University Press, 1960).

The application of the symmetry operators of the 11 Laue groups to the moments of order up to 6, results in sets of restrictions and algebraic equations for the components, that uniquely distinguish each group from the others. Since the moments are tensors, the symmetry restrictions have semi-invariant character and can be properly transferred into any other given reference system. Thus, each set of the above mathematical relationships can be used as semi-invariant descriptor of the group symmetry.

Considering the distribution of the intensities in the reciprocal space, a useful application of these results has been found in the characterisation of the three-dimensional diffraction patterns. Indeed it is possible to recognise the Laue symmetry of a data set as well as to check the departure of a data set from an assumed point group symmetry. Moreover, it is possible to determine the point group symmetry of the diffraction pattern of data affected by anomalous scattering.

The functional relations among the high-order moments' components in the various groups, with respect to both the conventional crystallographic axes and the internal reference system, will be presented and discussed.

MS-17.01.02 CRYSTALLOGRAPHIC POINT GROUPS OF FIVE-DIMENSIONAL SPACE

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The number of the Crystallographic Point Groups is well known in 2, 3 and 4-dimensional spaces. There are 10 in 2-dimensional space and 32 in 3-dimensional space which are characterized by the Hermann-Mauguin symbols. There are 227 in 4-dimensional space [1]. For these groups, we suggested geometrical WPV (Weigel, Phan, Veyseyre) symbols [2], [3] which generalize the Hermann-Mauguin symbols.

The determination of the Crystallographic Point Groups of 5-dimensional space started in the thesis of Th. Phan [4] for the crystal families which describe di-incommensurate structures; 90 Point Groups of this space have been described.

By means of numerical analysis and computer science, we found all the Crystallographic Point Groups of 5-dimensional space, i.e. all the subgroups of the different holohedries. At first, we suggested WPV symbols for the holohedries in connection with the geometrical construction of the crystal families and then, for all the Point Groups, by studying their elements or Point Symmetry Operations.

For instance, $\bar{1} \perp 4 m m$ is the WPV symbol of the holohedry of the "TRICLINIC SQUARE" family, its order is 16; its different subgroups are:

$m; 2; \bar{1}; \bar{1}_4$ of order 2

$4; \bar{1} \perp 2; \bar{1} \perp m; \bar{1}_4$ of order 4

$4 m m; \bar{1} \perp 4; 4, \bar{1}_4, \bar{1}_4; \bar{4}, m, \bar{1}_4$ of order 8

[1] BROWN, BÜLOV, NEUBÜSER, WONDRATSCHEK & ZASSENHAUS
Crystallographic Groups of four-dimensional Space John Wiley & Sons (1978)

[2] D. WEIGEL, T. PHAN & R. VEYSSEYRE *Acta Cryst.* (1987) A 43, 294-304

[3] R. VEYSSEYRE Thesis PARIS-VI (1987)

[4] T. PHAN Thesis PARIS-VI (1989)

MS-17.01.03 A SIMPLE ALGEBRA AND GEOMETRY IN THE 2-D PENROSE TILING By Hsueh-Hsing Hung, Synchrotron Radiation Research Center, Taiwan

A simple implication in 2-dimensional Penrose tilings with the global orientational symmetry is revealed in this talk. We will point out a plain relation between the definition of the generalized golden mean and the local matching geometry and propose an inflation rule to span the whole plane from a unit symmetric zone.