20.1-1   IRREDUCIBLE TENSORIAL METHOD FOR MAGNETIC CRYSTALS. FULL SET OF TABLES. By M.N. Angelova, M.I.Aroyo and J.N.Kotzev. Faculty of Physics, University of Sofia, Sofia-1126, Bulgaria

The method of irreducible tensorial sets (ITS) is generalized for systems with magnetic symmetry, based on the Wigner corepresentations (coreps) and the Shubnikov antiunitary point gpoups. The following basic results are obtained: (i) generalized Racah lemma by which the ITS of an antiunitary group can be built up from the ITS of its supergroup; (ii) new form of Wigner-Eckart theorem for coreps,by which the matrix elements of quantum mechanical operators in magnetic systems can be factorized, is given; (iii) the theory of building elements of ITS for coreps is developed and their properties are investigated. An effective method for calculation of ITS coefficients is developed on the base of generalized Racah lemma. The following coefficients for all single- and double-valued coreps of all 90 Shubnikov antiunitary magnetic point groups are tabulated: (i) Clebsch-Gordan coefficients (J.Phys.A(1981) 14,1543; (1982) 15,711; (1982) 15,725); (ii) symmetrized Clebsch-Gordan coefficients the so called 3D-symbols and 2D-symbols (J.Mol. Structures(1984), in press); (iii) isoscalar factors for all possible transitions between 90 magnetic point groups, where the coreps D^j of $O(3) \times \theta$ whith $j=0,1/2,1,...,3$ are used as starting coreps (Comm.Roy.Soc. Edinburgh (1983)19, 253); (iv) 6D-symbols.
The tables are available by request from the authors.

This contrasts with the situation in single crystals where there is only one mode of equivalence of crystal directions.

If the crystals are non-enantiomorphic, two modes of equivalence can nevertheless be defined in this case, too, by the definitions

$$\mathcal{F}_{yt}(h) = \mathcal{F}_y(h) \qquad \text{1 mode}$$
$$\mathcal{F}_{yt}(a^c \cdot h) = \mathcal{F}_y(h) \qquad \text{2 mode} \right\} \begin{array}{c} \text{of equivalence} \\ \text{(3 b)} \end{array}$$

where a^c is one of the symmetry operations of second kind, $|a^c_{ik}| = -1$, of the crystal symmetry.

The mode of equivalence is to be kept apart from the kind of the geometrical symmetry operation defined by the sign of $|a^s_{ik}|$ in eq. (1). The second mode of equivalence has the properties of a cyclic group of second order. The symmetry of a polycrystalline aggregate, defined by eq. (1) and (3) can thus be described by a black-white point group.

References:

H.J. Bunge, C. Esling and J. Muller: J. Appl. Cryst. (1980) 13, 544-554

H.J. Bunge, C. Esling and J. Muller: Acta Cryst. (1981) A 37, 889-899

20.1-2   SYMMETRY CLASSIFICATION OF POLYCRYSTALLINE AGGREGATES. By H.J. Bunge, Dep. of Physical Metallurgy, Univ. of Clausthal, FRG; and C. Esling, Dep. of Structural Metallurgy, Univ. of Metz, France

The symmetry description of single crystals by point groups must be generalized in order to take all possible point symmetries in polycrystalline aggregates into account.

A symmetry operation of an aggregate can be defined by a unitary transformation a^s transforming a unit vector $\vec{y}$, representative for a sample direction, into $\vec{y}^t$

$$\vec{y}^t = a^s \cdot \vec{y}, \quad |a^s_{ik}| = \pm 1, \quad \vec{y} = \{y_1, y_2, y_3\} \quad (1)$$

and the additional requirement that $\vec{y}$ and $\vec{y}^t$ be equivalent. Equivalence of two sample directions $\vec{y}$ and $\vec{y}^t$ in a polycrystalline aggregate is defined in a statistical sense by the distribution function $I_y(h)$ of crystal directions h which are parallel to the sample direction $\vec{y}$. This function is invariant with respect to all symmetry rotations of the crystal symmetry

$$\mathcal{F}_y(a^c \cdot h) = \mathcal{F}_y(h), \quad |a^c_{ik}| = +1 \quad (2)$$

If the crystals belong to an enantiomorphic class, then two such functions $I^R_{\vec{y}}(h)$ and $I^L_{\vec{y}}(h)$ are to be distinguished corresponding to right- and left-handed crystals respectively. Equivalence of two sample directions $\vec{y}$ and $\vec{y}^t$ in an aggregate can then be obtained in two different modes:

$$\mathcal{F}^R_{yt}(h) = \mathcal{F}^R_y(h), \ \mathcal{F}^L_{yt}(h) = \mathcal{F}^L_y(h) \quad \text{1 mode}$$
$$\mathcal{F}^R_{yt}(h) = \mathcal{F}^L_y(h), \ \mathcal{F}^L_{yt}(h) = \mathcal{F}^R_y(h) \quad \text{2 mode} \right\} \begin{array}{c} \text{of equivalence} \\ \text{(3a)} \end{array}$$

20.1-3   TO COMPLETING THE SCHEME OF THE 5-DIMENSIONAL CRYSTALLOGRAPHIC GROUPS OF SYMMETRY. By A.F.Palistrant, Dept. of Mathematics and Cybernatics, Kishnev State University, Kishnev, USSR.

The use of the methods [1,2] for employing the classical crystallographic groups of symmetry and their generalizations with the simple and 1-fold Shubnikov-Zamorzaev antisymmetry, p - and (p') - Belov-Pawley symmetry, and 32 crystallographic P-symmetries in geometrical classification (when the permutation group of the quality P is isomorphic to one in 32 crystallographic classes) to the count and modelling of the 4-dimensional groups of symmetry makes it possible to progress the principle solution of the n-dimensional geometric crystallography problem where n=5.

Indeed, the detailed calculations of the three-dimensional groups of symmetry and two-fold antisymmetry allow the numbers of the category $G_{543...t}$, groups to be found. There are 17410 G_{543}; 2597G_{5431}; 4920G_{5432}; 1379G_{54321}; 624 G_{5430}; 671G_{54320}; 374G_{543210} (in accordance with the full numbers of the groups of symmetry and two-fold antisymmetry G^2_3 and G^2_{31} (ignoring enantiomorphism); G^2_{32}; G^2_{321}; G^2_{30}; G^2_{320}; G^2_{3210}).

On the other hand, 5-dimensional crystallographic groups of the category $G_{53...t}$ can be found by the use of the 3-dimensional classic groups $G_{3...t}$ and their generalizations with antisymmetry, p- and (p')-symmetry (ignoring enantiomorphism), when p=2,3,4,6 (where only the groups of the full marked generalized symmetries are extracted). Thus, there are 33075 G_{53} (in accordance with the full numbers of the groups G_3, G_3^{4}, G_3^{p} and $G_3^{p'}$); 1208G_{530} (in accordance with the full numbers of the groups G_{30}, G_{30}^{4}, G_{30}^{p} and $G_{30}^{p'}$); 5177G_{531}; 9282G_{532}; 1274G_{5320}; 2597G_{5321}.

Finally, the groups of the categories G_{52} and G_{521} are fully discribed by the classical groups G_2 and G_{21} and their generalizations with the 31 nontrivial crystallographic P-symmetries in the geometric classification.

For the completion of the scheme of the 5-dimensional crystallographic groups of symmetry it is necessary to find the numbers of the groups of the categories G_5; G_{50}; G_{51}; G_{54} and G_{510}.

References.

1. A.M.Zamorzaev, A.F.Palistrant. Z.Kristallografia, 151, 231 (1980)
2. A.F.Palistrant.DAN SSSR,260,884(1981). In Russian.

20.1—4   DIFFRACTION GROUPS OF CBED PATTERNS.   By P.Goodman, Division of Chemical Physics, CSIRO, Australia.

Symmetry rules so far derived for CBED patterns can be summarised in the form of matrix generators operating in diffraction space, which contain the 2-dimensional rotation groups as a partioned component.

In contrast to the matrix representation of space groups in kinematic x-ray diffraction space (i.e. Fourier space: Beinstock,A. and Ewald,P.P,(1962),Acta Cryst. 15,1253) it is the di-periodic layer groups rather than the 3-dimensional space groups which are defined. This is a consequence of the substitution of parallel-plate boundary conditions for the restrictions imposed by Friedel's law in x-ray kinematic scattering.

As a result 80 groups, containing 43 symmorphic groups, can be defined in diffraction space. From these the previously-derived 31 CBED groups (Buxton,B.F. Eades,J.A.,Steeds,J.W.and Rackham,G.M.(1976), Phil.Trans. 281,171) emerge as the point-group component . It is therefore clear that the same boundary conditions have been assumed in this previous derivation as in the present one. The two systems are hence mutually consistent, the increased resolution of the new derivation coming from (a) the use of arithmetic rather than geometric definition for the rotation group and (b) the inclusion of dynamic extinctions of the zero layer.

20.1—5   THE METHOD OF MATRICAL REPRESENTATION OF CRYSTAL SYMMETRY GROUPS AND ITS POSSIBILITIES   By T.N.Liopo, V.A.Liopo. Brest pedagogical institute,Brest,Belorussia,USSR.

The correlations between macrosymmetry, the parameters of the unit cells and physical properties of crystals are analysed. An analitical method of construction and analysis of crystallographic projections is shown. It is developed the practical matrical method for mutual transition of crystal and reciprocal lattice. It is given the way of transference from one crystallographic basis to another and analysed the changes of crystallographic indexes of planes, directions and points in this case. It is proposed the method of matrical representation for symmetry groups of sets and layers, and the limited, gomothetical and black-white groups of crystals The results of culculations are compared to the experimental data got for some monoclinical (layer silicates) and cubical (semiconductors) crystals.

20.1—6   ON THE DIFFRACTION ENHANCEMENT OF SYMMETRY. By Hitoshi Iwasaki, The Institute of Physical and Chemical Research, Wako-shi, Saitama 351, Japan.

The point group symmetry of the weighted reciprocal lattice, or diffraction symmetry, can in some special cases be higher than the Laue-class symmetry of the crystal. When such a phenomenon occurs other than as a result of Friedel law, it is called diffraction enhancement of symmetry: for example, a triclinic crystal may produce monoclinic or orthorhombic diffraction patterns, and in fact several such cases have actually been recognized. Efforts to shed light on this problem have been made by many authors (Iwasaki, Acta Cryst. (1972) A28, 253; Perez-Mato et al., ibid. (1977) A33, 466; Sadanaga et al., ibid. (1979) A35, 115 and others), but the question to what extent the enhancement may occur has been left unsettled.

On examining structures (S) which show diffraction enhancement, some of them were found to be expressed by superposition of an average structure (A) and a few modulating structures (M). If both A and M are of higher symmetry than S, and in addition if each of A and M gives finite diffraction intensities at separate set of reciprocal lattice points (for example, only h=2n for A and only h=2n+1 for M), then the symmetry of overall diffraction pattern produced by S should conform to the symmetry of A and M, and not to that of S. By applying this principle to various combinations of the point groups of S, A and M, it is possible to conclude that every types of enhancement do occur at least mathematically. It means that when a diffraction group D corresponding to an unknown structure is arbitrarily given, the point group of S may be any subgroup of D.