

20.1-13 COLOUR SYMMETRY AND SCALLING IN PHASE TRANSITION AND CRITICAL PHENOMENA THEORY. By V.A.Koptsik, Moscow University, Moscow, USSR

It is shown that the method of generalized representations of the classical space and point groups, and the method of coloured  $P$  and  $Q$ -groups in their magnetic interpretation are the equivalent languages for the symmetry description of magnetic structures arising through the phase transitions in crystals. The colour symmetry methods may be effectively used in the theory of critical phenomena because the scaling transformations of the appropriate Hamiltonians are nothing but a special realization of the  $US \rightarrow EUC$ ,  $BZ \rightarrow RBZ$  transformations in the colour symmetry groups. The principal idea of colour scaling consists in the abstract symmetry conservation law for isolated physical systems. The commensurate (or incommensurate) modulated structure of a crystal arising through the phase transitions may be described in terms of colour space groups isomorphic (or homomorphic) to the initial space groups:

$$\Phi = TG = T^* \{t_i\} G = T^* G^{(t_i)} \leftrightarrow T^* G^{(t_i, w)} = T^{(w)} G^{(t_i, w)} = \Phi^{(w)} \subset P^{\Phi} \Phi.$$

We use there the non-standard factorization of the space group  $\Phi$  connected with the enlarged unit cell EUC and go to the isomorphic positional colour space group  $\Phi^{(w)} \leftrightarrow \Phi$  which is the subgroup of the wreath products of the groups  $P$  and  $\Phi$  which correspond to the selected model of imperfect crystal. The action of the generalized symmetry operators  $\langle p_i^{\Phi} | g_i \rangle \in G^{(t_i, w)} \leftrightarrow G^{(t_i)}$  on the field order parameter  $\eta(\vec{z})$  depends on the point coordinates  $\vec{z}_i = g_i \vec{z}$ ,  $g_i \in G^{(t_i, w)}$ . Averaging  $\eta(\vec{z})$  throughout the group  $G^{(t_i, w)}$  in the volume of EUC one obtains the uniform distribution of  $\eta = \langle \eta(\vec{z}) \rangle$ . To the scaling transformations  $US \rightarrow EUC$  there correspond the transformations from initial microscopic to some block Hamiltonian. If this result coincides with that of the renormalization group approach and with the experimental data one may take the test model of  $T^* G^{(t_i, w)} = \Phi^{(w)}$  group for the representative subgroup of the generalized microscopic symmetry of modulated phase of a crystal in the class of the equivalent symmetry groups. It follows from abstract symmetry conservation law that  $\Phi^{(w)}$  is isomorphic to the group  $\Phi_p$ , and that  $\Phi_p$  is the common subgroup of  $\Phi_p$  and  $\Phi_p^{(w)}$  in accordance with the experiment and theory of Landau.

20.2-1 APPLICATION OF EXPLICIT-ORIGIN SPACE GROUP NOTATION. By S.R. Hall, Crystallography Centre, University of Western Australia, Nedlands 6009, Australia.

The explicit-origin space group notation of Hall (Acta Cryst. (1981) A37, 517) has a number of advantages over the commonly-used short and full Hermann-Mauguin symbols for computer-based symmetry operations. Foremost, the new symbols are very simply translated into both site and reflection symmetry information. It has other important advantages as well. There is a clear relationship between space group symmetries related by an inversion centre (e.g.  $P22_{ab}$  and  $-P22_{ab}$  instead of  $P2_12_12$  and  $Pbam$ ) or by point groups (e.g.  $-P2_a2_a$  and  $-P2_a2_n$  instead of  $Pmma$  and  $Pbcn$ ); the facility for all possible axial settings with symbols which exhibit the same features; and a difference in notation when an inversion centre is not placed at the origin (e.g.  $-P4_a2_b$  and  $P42_1$  are the centrosymmetric and non-centrosymmetric forms of  $P4/nbm$ ).

The recent addition of an origin shift parameter to the notation provides for site compatibility with all previous (and future) space group settings. This, and the above features, make the explicit-origin symbols ideal for computer data-base and archival purposes. For this reason they have been adopted by the XTAL Program System (Hall et al., Acta Cryst. (1980) A36, 979) and the Standard Crystallographic File Structure (Brown, Acta Cryst. (1983) A39, 216). The origin shift update, the symbol translation algorithm and some applications will be described.

20.2-2 THE IMPLICATION OF EUCLIDEAN NORMALIZERS OF SPACE GROUPS ON INDICES AND PHASES OF STRUCTURE FACTORS. By E. Koch, Institute for Mineralogy, University of Marburg, Lahnberge, D-3550 Marburg, FRG.

The Euclidean normalizer  $N_E(G)$  of a space group  $G$  forms the appropriate tool to derive all equivalent descriptions of a crystal structure or its enantiomorph from a given one. For this, two different methods may be used:

(1) The space group (the location of its symmetry elements) and the unit cell (basis vectors and origin) are kept fixed in space, whereas the coordinates of all atoms are transformed by the symmetry operations of  $N_E(G)$  (W. Fischer & E. Koch, Acta Cryst. (1983) A39, 907). By this means the crystal structure or its enantiomorph is embedded into the unit cell in  $n$  different ways, each referring to one of the  $n$  cosets of  $G$  in  $N_E(G)$  and each giving rise to another coordinate description.

(2) The crystal structure itself and therewith its symmetry elements (the space group) are kept fixed in space, whereas the original chosen unit cell is transformed (rotated, inverted, translated) by the symmetry operations of  $N_E(G)$ . This procedure results in the same  $n$  coordinate descriptions as method (1), but the transition to the enantiomorph is replaced by the change of the handedness of the basis system.

For studying the implication of Euclidean normalizers in reciprocal space the second approach is more adequate: Each change of coordinate system in direct space, described by a matrix-vector pair  $(P, p)$ , causes a basis transformation in reciprocal space and, as a consequence, a change of indices for all reflections from  $h$  to  $h' = hP$  and of structure-factor phases from  $\varphi(h)$  to  $\varphi'(h') = \varphi(h) - 2\pi hp$  (for symbolism cf. H. Arnold in: International Tables for Crystallography, Vol. A (1983) D. Reidel). If  $(P, p)$  corresponds to a symmetry operation of  $G$  itself, the original set of indices and related