

20.1-3 THE APPLICATION OF EIGENSYMMETRIES OF FACE FORMS TO X-RAY DIFFRACTION PROBLEMS. By H. Klapper and Th. Hahn, Institut fuer Kristallographie der RWTH, D-5100 Aachen, Federal Republic of Germany.

A face form (crystal form)  $\{hkl\}$  is a polyhedron (closed or open) which consists of all faces equivalent to a given face  $\{hkl\}$  with respect to a (generating) point group. Each face form has a well-defined *eigensymmetry* which is a proper or improper supergroup of the generating symmetry (Th. Hahn and H. Klapper, Internat. Tables for Crystallogr., Vol. A, p. 755, 771. Reidel, 1983). Among the 47 different face forms, 22 have centrosymmetric and 25 non-centrosymmetric *eigensymmetries*. Example: The rhombohedron  $\{h\bar{0}h\}$  has the centrosymmetric *eigensymmetry*  $\bar{3}m$ , one possible generating symmetry is the non-centrosymmetric point group  $32$ .

In 'monoaxial' point groups (e.g.  $4$ ,  $\bar{6}$ ,  $6/m$ ) the orientation of the *eigensymmetry* elements of a face form  $\{hkl\}$  coincides only for special values of  $h, k, l$  with the orientation of the symmetry elements of the lattice (holohedry). Example: In point group  $6$  all hexagonal prisms  $\{hk\bar{l}0\}$  have the same *eigensymmetry* but different orientations (for short: different 'oriented' *eigensymmetries*).

*Eigensymmetries* of face forms are useful for certain diffraction problems related to anomalous scattering and twinning by merohedry. For this purpose, the face form  $\{hkl\}$  corresponding to an X-ray reflection  $hkl$  is considered.

(a) Friedel-pair reflections in the presence of anomalous scattering:

For non-centrosymmetric crystals with anomalous scatterers, Friedel's rule is not violated for certain reflections. These can easily be determined by the following rule:

In the presence of anomalous scattering, Friedel's rule, i.e.  $I(hkl) = I(\bar{h}\bar{k}\bar{l})$ , is strictly valid for a reflection  $hkl$ , if the *eigensymmetry* of the corresponding face form  $\{hkl\}$  is centrosymmetric; it is violated if the *eigensymmetry* of  $\{hkl\}$  is non-centrosymmetric.

(b) X-ray intensities of crystals twinned by merohedry: For twinning by merohedry the lattices of the twin domains are exactly parallel, i.e. for any reflection  $hkl$ , all domains are in reflection position. With respect to the intensities, however, two types of reflections, (1) and (2), are distinguished by the following criterion: (1) The twin element belongs to the 'oriented' *eigensymmetry*, (2) the twin element does not belong to the 'oriented' *eigensymmetry* of the face form  $\{hkl\}$ .

The following rule can be deduced:

For type (1) reflections all domain variants have the same intensity, with or without anomalous scattering. For type (2) reflections the intensity differs for different domain variants, again with or without anomalous scattering, except for twinning by inversion.

If the twin element is the inversion, or if the combination of twin element and *eigensymmetry* of the face form  $\{hkl\}$  contains the inversion, type (2) reflections require special consideration: They exhibit equal intensities for both domain variants in the absence of anomalous scattering (due to Friedel's law) and different intensities in the presence of anomalous scattering.

Rule b) implies that the intensities of type (1) reflections are not affected by the twinning and are the same for twinned and untwinned crystals, whereas for type (2) reflections the intensity depends on the relative proportions of the domain variants. The rule is particularly useful in structure determinations of crystals twinned by merohedry. Another application is found in X-ray topography of twinned crystals, where twin domains can be imaged if reflections of type (2) are used. This will be illustrated by topographs of twinned  $KLiSO_4$ ,  $NaLiSO_4$ , and quartz crystals.

20.2-1 THE NON-CHARACTERISTIC ORBITS OF THE PLANE GROUPS. By T. Matsumoto, Dept. of Earth Sciences, Faculty of Science, Kanazawa University, Kanazawa, 920 Japan; H. Wondratschek, Institut für Kristallographie der Universität Karlsruhe (TH), 7500 Karlsruhe, BRD.

The set of all points which are symmetrically equivalent to a point  $X$ , with respect to a plane group  $G$  is called the  $G$ -orbit,  $GX$  of  $X$ . The set of all isometries leaving the  $G$ -orbit invariant is called the *eigensymmetry* plane group  $C$  of  $GX$ .  $C \cong G$  holds. The  $G$ -orbit is characteristic if  $G = C$ , and non-characteristic if  $G < C$ .

A complete listing of non-characteristic  $G$ -orbits for the space groups, with the limits of the same crystal family of  $G$  and  $C$ , has been published (Engel, Matsumoto, Steinmann and Wondratschek, Zeit. Krist., Supplement 1, 1984, 1-218).

By means of group-subgroup relations, all non-characteristic  $G$ -orbits of the plane groups have been derived and listed, i.e. all the  $G$ -orbits, whose Euclidean stabilizer  $C$  (*eigensymmetry* plane groups) exceeds  $G$ ;  $C > G$ , by Matsumoto and Wondratschek independently. The lists derived for the plane contain also the non-characteristic orbits without restriction of the same crystal family of  $G$  and  $C$ . The pair of eigen plane group and eigen site symmetry is called the *eigenaspect* of the  $G$ -orbit  $GX$  of  $X$ . A type of aspects that contains at least one *eigenaspect* is called  $E$ -type of aspects. There are 30  $E$ -types of aspects. The relations between 30  $E$ -types of aspects of the plane can also be shown by specialization for the five parameters ( $x, y, a, b, \gamma$ ). 13  $E$ -types of aspects can not be obtained from another type of aspects by specialization (13 essential different kinds of regular systems of points (Sohncke, 1874)). There are 7  $E$ -types of aspects which can not be specialized to others with less parameters.

20.3-1 LATTICE SITES AND NMR CHEMICAL SHIFTS IN SILICON CARBIDE POLYTYPES. By Mary Frances Richardson, J. Stephen Hartman, Barbara L. Sherriff, and Beatrice G. Winsborrow, Department of Chemistry, Brock University, St. Catharines, Ontario L2S 3A1, Canada.

Silicon carbide polytypes give distinctive  $^{29}\text{Si}$  and  $^{13}\text{C}$  Magic Angle Spinning nmr spectra which can be related to the number and types of lattice sites present. A local-site designation system is developed for lattice sites in silicon carbide polytypes and related to  $^{29}\text{Si}$  and  $^{13}\text{C}$  chemical shifts. Only four kinds of lattice sites are possible when surroundings out of 5A are considered, and two of these must be present in equal numbers regardless of polytype. If surroundings beyond 5A are considered, the number of distinctive lattice sites increases in long-C-axis polytypes.  $^{29}\text{Si}$  and  $^{13}\text{C}$  chemical shifts of silicon carbide are related in an intriguing "mirror image" fashion, and insights gained from chemical shift calculations will be discussed.