International Tables for Crystallography (2006). Vol. A1, Section 1.1.4, pp. 4–5.

structures are found in Neubüser & Wondratschek (1966). In the early tables, the subgroups were only listed by their types. For *International Tables*, an extended list of maximal non-isomorphic subgroups was prepared. For each space group the maximal *translationengleiche* subgroups and those maximal *klassengleiche* subgroups for which the reduction of the translations could be described as 'loss of centring translations' of a centred lattice are listed individually. For the other maximal *klassengleiche* subgroups, *i.e.* those for which the conventional unit cell of the subgroup is larger than that of the original space group, the description by type was retained, because the individual subgroups of this kind were not completely known in 1983. The deficiency of such a description becomes clear if one realizes that a listed subgroup type may represent 1, 2, 3, 4 or even 8 individual subgroups.

In the present Volume A1, *all* maximal non-isomorphic subgroups are listed individually, in Chapter 2.2 for the plane groups and in Chapters 2.3 and 3.2 for the space groups. In addition, graphs for the *translationengleiche* subgroups (Chapter 2.4) and for the *klassengleiche* subgroups (Chapter 2.5) supplement the tables. After several rounds of checking by hand and after comparison with other listings, *e.g.* those by H. Zimmermann (unpublished) or by Neubüser and Eick (unpublished), intensive computer checking of the hand-typed data was carried out by F. Gähler as described in Chapter 1.4.

The mathematician G. Nebe describes general viewpoints and new results in the theory of subgroups of space groups in Chapter 1.5.

The maximal *isomorphic* subgroups are a special subset of the maximal *klassengleiche* subgroups. Maximal isomorphic subgroups are treated separately because each space group $\mathcal{G}$ has an infinite number of maximal isomorphic subgroups and, in contrast to non-isomorphic subgroups, there is no limit for the index of a maximal isomorphic subgroup of $\mathcal{G}$.

An *isomorphic subgroup* of a space group seems to have first been described in a crystal–chemical relation when the crystal structure of Sb_2ZnO_6 (structure type of tapiolite, Ta_2FeO_6) was determined by Byström *et al.* (1941): 'If no distinction is drawn between zinc and antimony, this structure appears as three cassiterite-like units stacked end-on-end' (Wyckoff, 1965). The space group of Sb_2ZnO_6 is a maximal isomorphic subgroup of index 3 with $\mathbf{c}' = 3\mathbf{c}$ of the space group $P4_2/mnm$ (D_{4h}^{14}, No. 136) of cassiterite SnO_2 (rutile type).

The first systematic study attempting to enumerate all isomorphic subgroups (not just maximal ones) for each space-group type was by Billiet (1973). However, the listing was incomplete and, moreover, in the case of enantiomorphic pairs of space-group types, only those with the same space-group symbol (called *isosymbolic space groups*) were taken into account.

Sayari (1976) derived the conventional bases for all maximal isomorphic subgroups of all plane groups. The general laws of number theory which underlie these results for plane-group types $p4$, $p3$ and $p6$ and space-group types derived from point groups 4, $\overline{4}$, $4/m$, 3, $\overline{3}$, 6, $\overline{6}$ and $6/m$ were published by Müller & Brelle (1995). Bertaut & Billiet (1979) suggested a new analytical approach for the derivation of all isomorphic subgroups of space and plane groups.

Because of the infinite number of maximal isomorphic subgroups, only a few representatives of lowest index are listed in *IT* A with their lattice relations but without origin specification, *cf.* *IT* A (2002), Section 2.2.15.2. Part 13 of *IT* A (Billiet & Bertaut, 2002) is fully devoted to isomorphic subgroups, *cf.* also Billiet (1980) and Billiet & Sayari (1984).

In this volume, all maximal isomorphic subgroups are listed as members of infinite series, where each individual subgroup is specified by its index, its generators and the coordinates of its conventional origin as parameters.

The relations between a space group and its subgroups become more transparent if they are considered in connection with their normalizers in the affine group $\mathcal{A}$ and the Euclidean group $\mathcal{E}$ (Koch, 1984). Even the corresponding normalizers of Hermann's group $\mathcal{M}$ play a role in these relations, *cf.* Wondratschek & Aroyo (2001).

In addition to subgroup data, supergroup data are listed in *IT* A. If $\mathcal{H}$ is a maximal subgroup of $\mathcal{G}$, then $\mathcal{G}$ is a minimal supergroup of $\mathcal{H}$. In *IT* A, the type of a space group $\mathcal{G}$ is listed as a minimal non-isomorphic supergroup of $\mathcal{H}$ if $\mathcal{H}$ is listed as a maximal non-isomorphic subgroup of $\mathcal{G}$. Thus, for each space group $\mathcal{H}$ one can find in the tables the types of those groups $\mathcal{G}$ for which $\mathcal{H}$ is listed as a maximal subgroup. The supergroup data of *IT* A1 are similarly only an inversion of the subgroup data.

1.1.4. Applications of group–subgroup relations

Phase transitions. In 1937, Landau introduced the idea of the *order parameter* for the description of *second-order phase transitions* (Landau, 1937). Landau theory has turned out to be very useful in the understanding of phase transitions and related phenomena. Such a transition can only occur if there is a group–subgroup relation between the space groups of the two crystal structures. Often only the space group of one phase is known (usually the high-temperature phase) and subgroup relations help to eliminate many groups as candidates for the unknown space group of the other phase. Landau & Lifshitz (1980) examined the importance of group–subgroup relations further and formulated two theorems regarding the index of the group–subgroup pair. The significance of the subgroup data in second-order phase transitions was also pointed out by Ascher (1966, 1967), who formulated the *maximal-subgroup rule*: 'The symmetry group of a phase that arises in a ferroelectric transition is a maximal polar subgroup of the group of the high-temperature phase.' There are analogous applications of the maximal-subgroup rule (with appropriate modifications) to other types of continuous transitions.

The group-theoretical aspects of Landau theory have been worked out in great detail with major contributions by Birman (1966*a*,*b*), Cracknell (1975), Stokes & Hatch (1988), Tolédano & Tolédano (1987) and many others. For example, Landau theory gives additional criteria based on thermodynamic arguments for second-order phase transitions. The general statements are reformulated into group-theoretical rules which permit a phase-transition analysis without the tedious algebraic treatment involving high-order polynomials. The necessity of having complete subgroup data for the space groups for the successful implementation of these rules was stated by Deonarine & Birman (1983): '... there is a need for tables yielding for each of the 230 three-dimensional space groups a complete lattice of decomposition of all its subgroups.' Domain-structure analysis (Janovec & Přívratská, 2003) and symmetry-mode analysis (Aroyo & Perez-Mato, 1998) are further aspects of phase-transition problems where group–subgroup relations between space groups play an essential role. Domain structures are also considered in Section 1.2.7.

In treating successive phase transitions within Landau theory, Levanyuk & Sannikov (1971) introduced the idea of a hypothetical parent phase whose symmetry group is a supergroup of the observed (initial) space group. Moreover, the detection of pseudosymmetries is necessary for the prediction of higher-temperature phase transitions, *cf.* Kroumova *et al.* (2002) and references therein.

In a reconstructive phase transition, there is no group–subgroup relation between the symmetries of the two structures. Nevertheless, it has been pointed out that the 'transition path' between the two structures may involve an intermediate unstable structure whose space group is a common subgroup of the space groups of the two phases (Sowa, 2001; Stokes & Hatch, 2002).

Overlooked symmetry. In recent times, the number of crystal-structure determinations with a wrongly assigned space group has been increasing (Baur & Kassner, 1992; Marsh *et al.*, 2002). Frequently, space groups with too low a symmetry have been chosen. In most cases, the correct space group is a supergroup of the space group that has been assigned. A criterion for the correct assignment of the space group is given by Fischer & Koch (1983). Computer packages for treating the problem can be made more efficient if the possible supergroups are known.

Twinning can also lead to a wrong space-group assignment if it is not recognized, as a twinned crystal can feign a higher or lower symmetry. The true space group of the correct structure is usually a supergroup or subgroup of the space group that has been assumed (Nespolo & Ferraris, 2004).

Relations between crystal structures. Working out relations between different crystal structures with the aid of crystallographic group–subgroup relations was systematically developed by Bärnighausen (1980). The work became more widely known through a number of courses taught in Germany and Italy from 1976 to 1996 (in 1984 as a satellite meeting to the Congress of the International Union of Crystallography). For a script of the 1992 course, see Chapuis (1992). The basic ideas can also be found in the textbook by Müller (1993).

According to Bärnighausen, a family tree of group–subgroup relations is set up. At the top of the tree is the space group of a simple, highly symmetrical structure, called the *aristotype* by Megaw (1973) or the *basic structure* by Buerger (1947, 1951). The space groups of structures resulting from distortions or atomic substitutions (the *hettotypes* or *derivative structures*) are subgroups of the space group of the aristotype. Apart from many smaller Bärnighausen trees, some trees that interrelate large numbers of crystal structures have been published, *cf.* Section 1.3.1. Such trees may even include structures as yet unknown, *i.e.* the symmetry relations can also serve to predict new structure types that are derived from the aristotype; in addition, the number of such structure types can be calculated for each space group of the tree (McLarnan, 1981*a*,*b*,*c*; Müller, 1992, 1998, 2003).

Setting up a Bärnighausen tree not only requires one to find the group–subgroup relations between the space groups involved. It also requires there to be an exact correspondence between the atomic positions of the crystal structures considered. For a given structure, each atomic position belongs to a certain Wyckoff position of the space group. Upon transition to a subgroup, the Wyckoff position will or will not split into different Wyckoff positions of the subgroup. With the growing number of applications of group–subgroup relations there had been an increasing demand for a list of the relations of the Wyckoff positions for every group–subgroup pair. These listings are accordingly presented in Part 3 of this volume.

references