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.'

The group–subgroup relations between space groups are fundamental for the so-called symmetry-mode analysis of phase transitions that allows the determination of the contributions of the primary and secondary order parameters to the structural distortion characterizing the transition (Aroyo & Perez-Mato, 1998). 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 number of cases, transitions between two phases with no group–subgroup relations between their space groups have been analysed using common subgroups. For examples, see Sections 1.6.4.5 and 1.7.3.1.5.

Domain structures and twinning. Domain-structure analysis (Janovec & Přívratská, 2003; Janovec *et al.*, 2003) is another aspect of phase-transition problems where group–subgroup relations between space groups play an essential role. The mutual orientations of twin domains resulting from phase transitions involving a group–subgroup relation can be derived. This is also an aid in the crystal-structure determination of twinned crystals. Domain structures are considered in Sections 1.2.7 and 1.6.6.

Topotactic reactions. Bernal (1938) observed that in the solid-state reaction $Mn(OH)_2 \rightarrow MnOOH \rightarrow MnO_2$ the starting and the product crystal had the same orientation. Chemical reactions in the solid state are now called topotactic reactions if the crystal orientations of the reactant and the product(s) are related (Giovanoli & Leuenberger, 1969; Lotgering, 1959). Frequently, like in the case of phase transitions, the space groups of the reactant and the product(s) are connected by a group–subgroup relation which allows one to explain the domain structure of the product crystals. *cf.* Sections 1.6.2 and 1.6.6.

Overlooked symmetry. Since powerful diffractometers and computer programs for crystal-structure determination have become widespread and easy to handle, the number of crystal-structure determinations with a wrongly assigned space group has been increasing (Baur & Kassner, 1992; Clemente, 2005; Marsh *et al.*, 2002; Marsh & Clemente, 2007). 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).

Solution of the phase problem. Group–subgroup relations can be of help in solving the phase problem in the crystal-structure determination of proteins (Di Costanzo *et al.*, 2003).

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, France and Italy from 1976 to 2008. For a script of the 1992 course, see Chapuis (1992). The script of the 2008 course is available at http://www.crystallography.fr/mathcryst/gargnano2008.htm. The basic ideas can also be found in the textbook by Müller (2006). For a review see Müller (2004). Details are presented in Chapter 1.6.

Prediction of crystal structures. Bärnighausen trees (see Chapter 1.6) 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, *cf.* Section 1.6.4.7. In addition, the number of such structure types can be calculated for each space group of the tree.

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 immediate 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.

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