International Tables for Crystallography (2006). Vol. A1, Section 1.2.7.1, pp. 18–19.

union $\mathcal{T}_g \cup (\mathcal{T}_g\,(t_a\,\overline{\mathbf{1}}_0))$. There are thus two maximal isomorphic subgroups of index 2 which are obtained by doubling the a lattice parameter. There are altogether 14 isomorphic subgroups of index 2 for any space group of type $P\,\overline{1}$ which are obtained by seven different cell enlargements.

If $\mathcal{G}$ belongs to a pair of enantiomorphic space-group types, then the isomorphic subgroups of $\mathcal{G}$ may belong to different crystallographic space-group types with different HM symbols and different space-group numbers. In this case, an infinite number of subgroups belong to the crystallographic space-group type of $\mathcal{G}$ and another infinite number belong to the enantiomorphic space-group type.

Example 1.2.6.2.7.

Space group $P4_1$, No. 76, has for any prime number $p > 2$ an isomorphic maximal subgroup of index p with the lattice parameters $a,\ b,\ pc$. This is an infinite number of subgroups because there is an infinite number of primes. The subgroups belong to the space-group type $P4_1$ if $p \equiv 1 \bmod 4$; they belong to the type $P4_3$ if $p \equiv 3 \bmod 4$.

Definition 1.2.6.2.8. A subgroup of a space group is called *general* or a *general subgroup* if it is neither a *translationengleiche* nor a *klassengleiche* subgroup. It has lost translations as well as linear parts, *i.e.* point-group symmetry. □

Example 1.2.6.2.9.

The subgroup $\mathcal{T}_g$ in Example 1.2.6.2.6 has lost all inversions of the original space group $P\overline{1}$ as well as all translations with odd u. It is a general subgroup $P1$ of the space group $P\overline{1}$ of index 4.

1.2.6.3. *The role of normalizers for group–subgroup pairs of space groups*

In Section 1.2.4.5, the normalizer $\mathcal{N}_{\mathcal{G}}(\mathcal{H})$ of a subgroup $\mathcal{H} < \mathcal{G}$ in the group $\mathcal{G}$ was defined. The equation $\mathcal{H} \trianglelefteq \mathcal{N}_{\mathcal{G}}(\mathcal{H}) \leq \mathcal{G}$ holds, *i.e.* $\mathcal{H}$ is a normal subgroup of $\mathcal{N}_{\mathcal{G}}(\mathcal{H})$. The normalizer $\mathcal{N}_{\mathcal{G}}(\mathcal{H})$, by its index in $\mathcal{G}$, determines the number $N_j = |\mathcal{G} : \mathcal{N}_{\mathcal{G}}(\mathcal{H})|$ of subgroups $\mathcal{H}_j < \mathcal{G}$ that are conjugate in the group $\mathcal{G}$, *cf.* Remarks (2) and (3) below Definition 1.2.4.5.1.

The group–subgroup relations between space groups become more transparent if one looks at them from a more general point of view. Space groups are part of the general theory of mappings. Particular groups are the *affine group* $\mathcal{A}$ of all reversible affine mappings, the *Euclidean group* $\mathcal{E}$ of all isometries, the *translation group* $\mathcal{T}$ of all translations and the *orthogonal group* $\mathcal{O}$ of all orthogonal mappings.

Connected with any particular space group $\mathcal{G}$ are its group of translations $\mathcal{T}(\mathcal{G})$ and its point group $\mathcal{P}_{\mathcal{G}}$. In addition, the normalizers $\mathcal{N}_{\mathcal{A}}(\mathcal{G})$ of $\mathcal{G}$ in the affine group $\mathcal{A}$ and $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ in the Euclidean group $\mathcal{E}$ are useful. They are listed in Section 15.2.1 of *IT* A. Although consisting of isometries only, $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ is not necessarily a space group, see the paragraph below Lemma 1.2.7.2.6.

For the group–subgroup pairs $\mathcal{H} < \mathcal{G}$ the following relations hold:

(1) $\mathcal{T}(\mathcal{H}) \leq \mathcal{H} \leq \mathcal{N}_{\mathcal{G}}(\mathcal{H}) \leq \mathcal{G} \leq \mathcal{N}_{\mathcal{E}}(\mathcal{G}) < \mathcal{E}$;

  (1*a*) $\mathcal{H} \leq \mathcal{N}_{\mathcal{G}}(\mathcal{H}) \leq \mathcal{N}_{\mathcal{E}}(\mathcal{H}) < \mathcal{E}$;

  (1*b*) $\mathcal{N}_{\mathcal{E}}(\mathcal{H}) \leq \mathcal{N}_{\mathcal{A}}(\mathcal{H}) < \mathcal{A}$;

(2) $\mathcal{T}(\mathcal{H}) \leq \mathcal{T}(\mathcal{G}) < \mathcal{T} < \mathcal{E}$;

(3) $\mathcal{T}(\mathcal{G}) \leq \mathcal{G} \leq \mathcal{N}_{\mathcal{E}}(\mathcal{G}) \leq \mathcal{N}_{\mathcal{A}}(\mathcal{G}) < \mathcal{A}$.

The subgroup $\mathcal{H}$ may be a *translationengleiche* or a *klassengleiche* or a general subgroup of $\mathcal{G}$. In any case, the normalizer $\mathcal{N}_{\mathcal{G}}(\mathcal{H})$ determines the length of the conjugacy class of $\mathcal{H} < \mathcal{G}$, but it is not feasible to list for each group–subgroup pair $\mathcal{H} < \mathcal{G}$ its normalizer $\mathcal{N}_{\mathcal{G}}(\mathcal{H})$. Indeed, it is only necessary to list for any space group $\mathcal{H}$ its normalizer $\mathcal{N}_{\mathcal{E}}(\mathcal{H})$ in the Euclidean group $\mathcal{E}$ of all isometries, as is done in *IT* A, Section 15.2.1. From such a list the normalizers for the group–subgroup pairs can be obtained easily, because for any chain of space groups $\mathcal{H} < \mathcal{G} < \mathcal{E}$, the relations $\mathcal{H} \leq \mathcal{N}_{\mathcal{G}}(\mathcal{H}) \leq \mathcal{G}$ and $\mathcal{H} \leq \mathcal{N}_{\mathcal{G}}(\mathcal{H}) \leq \mathcal{N}_{\mathcal{E}}(\mathcal{H})$ hold. The normalizer $\mathcal{N}_{\mathcal{G}}(\mathcal{H})$ consists consequently of all those isometries of $\mathcal{N}_{\mathcal{E}}(\mathcal{H})$ that are also elements of $\mathcal{G}$, *i.e.* that belong to the intersection $\mathcal{N}_{\mathcal{E}}(\mathcal{H}) \cap \mathcal{G}$, *cf.* the examples of Section 1.2.7.[10]

The isomorphism type of the Euclidean normalizer $\mathcal{N}_{\mathcal{E}}(\mathcal{H})$ may depend on the lattice parameters of the space group (*specialized* Euclidean normalizer). For example, if the lattice of the space group $P\overline{1}$ of a triclinic crystal is accidentally monoclinic at a certain temperature and pressure or for a certain composition in a continuous solid-solution series, then the Euclidean normalizer of this space group belongs to the space-group types $P2/m$ or $C2/m$, otherwise it belongs to $P\overline{1}$. Such a *specialized Euclidean normalizer* (here $P2/m$ or $C2/m$) may be distinguished from the *typical Euclidean normalizer* (here $P\overline{1}$), for which the lattice of $\mathcal{H}$ is not more symmetric than is required by the symmetry of $\mathcal{H}$. The specialized Euclidean normalizers were first listed in the 5th edition of *IT* A (2002), Section 15.2.1.

1.2.7. Application to domain structures

1.2.7.1. *Introductory remarks*

In this section, the group-theoretical aspects of domain (twin) formation (domain structure, transformation twin) from a homogeneous single crystal (phase **A**, parent phase) to a crystalline phase **B** (daughter phase, deformed phase) are discussed, where the space group $\mathcal{H}$ of phase **B** is a subgroup of the space group $\mathcal{G}$ of phase **A**, $\mathcal{H} < \mathcal{G}$. This happens, *e.g.*, in a displacive or order–disorder phase transition. In most cases phase **B**, the *domain structure*, is inhomogeneous, consisting of homogeneous regions which are called *domains*, defined below.

Only the basic group-theoretical relations are considered here. A deeper discussion of domain structures and their properties needs methods using representation theory, thermodynamic points of view (Landau theory), lattice dynamics and tensor properties of crystals. Such treatments are beyond the scope of this section. A detailed discussion of them is given by Tolédano *et al.* (2003) and by Janovec & Přívratská (2003).

In order to make the group-theoretical treatment possible, the *parent-clamping approximation*, abbreviated PCA, is introduced, by which the lattice parameters of phase **A** are not allowed to change at and after the transition to phase **B**, *cf.* Janovec & Přívratská (2003). Under the assumption of the PCA, two essential conditions hold:

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[10] For *maximal* subgroups, a calculation of the conjugacy classes is not necessary because these are indicated in the subgroup tables of Part 2 of this volume by braces to the left of the data sets for the low-index subgroups and by text for the series of isomorphic subgroups. For non-maximal subgroups, the conjugacy relations are not indicated but can be calculated in the way described here. They are also available online on the Bilbao crystallographic server, http://www.cryst.ehu.es/, under the program *Subgroupgraph*.

(1) The translations of phase **B** are translations of phase **A**. Thus, the space group $\mathcal{H}$ of **B** is a subgroup of the space group $\mathcal{G}$ of **A**, $\mathcal{H} < \mathcal{G}$. Without the PCA, the translations of **B** would not be translations of **A** and, therefore, **H** would not be a subgroup of **G**.

(2) Under the PCA, the more complicated ferroelastic phases[11] display the same simple behaviour as the non-ferroelastic ones. Disturbances which otherwise would be caused in ferroelastic phase transitions do not appear because there is no spontaneous strain.

The domain walls, *i.e.* the boundaries which separate different domains, will not be treated here because their symmetries are layer groups which are two-periodic groups in three-dimensional space and not space groups with three-dimensional periodicity. Layer groups are described in *International Tables for Crystallography*, Vol. E (2002).

Under these assumptions the domains formed may exhibit different chiralities and polarities of their structures and different spatial orientations of their symmetry elements, but each domain has the same specific energy and the lattice of each domain is part of the lattice of the parent structure **A** with space group $\mathcal{G}$.

In the discussion of domain structures, the following basic concepts are established: domain, domain state, symmetry state, orientation state. These concepts are defined and then applied in different examples of phase transitions in which the group-theoretical procedures and their results are explained.

The second step, the physically realistic situation at a temperature $T_x < T_C$ with the removal of the PCA, is only partly considered in this section. The relaxation of the PCA does not change the relations in a non-ferroelastic phase because all crystal regions suffer the same affine deformation. On the other hand, in ferroelastic phases the different spontaneous strains complicate the relations.

1.2.7.2. *Domains, domain states and symmetry states*

In a (continuous) phase transition with the symmetry reduction of the space group $\mathcal{G}$ to a subgroup $\mathcal{H} < \mathcal{G}$, a splitting of the parent phase **A** into many crystals of the type **B** is observed. The number of such crystals of **B** is not limited; they differ in their locations in space, in their orientations, in their shapes and in their space groups which, however, all belong to the same space-group type. In order to describe what happens in such a transition, a few notions are useful. If not explicitly stated, the validity of the PCA is assumed.

Definition 1.2.7.2.1. A connected homogeneous part of a domain structure or of a twinned crystal with structure type **B** is called a *domain*. Each domain is a single crystal. The part of the space that is occupied by a domain is the *region* of that domain. ☐

If the domains of phase **B** have been formed from a single crystal of phase **A**, then relations between the domains exist which are determined by group theory. In particular, the domains belong to a finite (small) number of domain states which have well defined relations to the original crystal **A** and its space group $\mathcal{G}$. In order to describe the relation of **B** to **A**, the notion of crystal pattern is used. Any perfect (ideal) crystal is a finite block of the corresponding infinite arrangement, the symmetry of which is a space group which contains translations. Here, this (infinite) periodic object is called a *crystal pattern*, *cf.* Section 1.2.2.1.

Definition 1.2.7.2.2. Two domains belong to the same *domain state* if their crystal patterns are identical, *i.e.* if they occupy different regions of space that are part of the *same* crystal pattern. In other words: a domain state is a crystal pattern. ☐

The number of domain states which are observed after a phase transition is limited and determined by the space groups $\mathcal{G}$ and $\mathcal{H}$. The number of domains which belong to the same domain state is not limited. The diversity of the domains and their shapes is due to mechanical stresses, defects, electrical charges and nucleation phenomena which strongly influence the kinetics of the phase transition.

A trivial domain structure is formed when phase **B** consists of one domain only, *i.e.* when it forms a *single-domain structure*. This is possible, in particular under an external electric field or under external stress. Such a procedure is known as ‘detwinning’. The corresponding domain state is a *single-domain state*. For a phase transition of the type considered, there are always several single-domain states which have the same *a priori* probability of appearing after a phase transition. In reality not all of them will be observed and/or their relative frequencies and sizes will be rather different.

Single-domain states are introduced in theoretical considerations in order to avoid the complications which may be caused by the coexistence of domains with different spontaneous strain in ferroelastic crystals of the structure **B** if the PCA cannot be assumed. In polydomain structures, the domains would distort or rotate each other a little and thus disturb the simple relations described now. These disturbances do not occur in non-ferroelastic transitions, so for them the simple relations also hold in polydomain structures without the PCA.

Lemma 1.2.7.2.3. The number Z of possible domain states after a phase transition under the PCA is equal to the index i of $\mathcal{H}$ in $\mathcal{G}$, $Z = |\mathcal{G} : \mathcal{H}| = [i]$. Let $\mathcal{G} = \mathcal{H}_1 \cup \ldots \cup g_j\mathcal{H}_1 \cup \ldots \cup g_i\mathcal{H}_1$ be the coset decomposition of $\mathcal{G}$ relative to $\mathcal{H}_1$, where $g_1 = e, \ldots, g_i$ are the coset representatives, and $\mathcal{H}_1$ is the space group of the domain state $\mathbf{B}_1$. The other domain states are obtained from $\mathbf{B}_1$ by $\mathbf{B}_k = g_k\mathbf{B}_1$, $k = 2, \ldots, i$. For the space group $\mathcal{H}_k$ of the domain state $\mathbf{B}_k$ the following holds: $\mathcal{H}_k$ is obtained by conjugation of the space group $\mathcal{H}_1$ of $\mathbf{B}_1$ with the same element g_k: $\mathcal{H}_k = g_k\mathcal{H}_1 g_k^{-1}$. ☐

If in a group–subgroup relation $\mathcal{G} > \mathcal{H}_q$ with index i_q the subgroups $\mathcal{H}_q$ belong to more than one conjugacy class, then each conjugacy class corresponds to a separate phase transition $\mathbf{A} \longrightarrow \mathbf{B}_k^{(1)}$, $\mathbf{A} \longrightarrow \mathbf{B}_k^{(2)}$ *etc*. These different phase transitions lead to different low-symmetry structures $\mathbf{B}^{(m)}$, have different transition temperatures and different probabilities of happening.

There are more elements of the group $\mathcal{G}$ than just g_k that map the domain state $\mathbf{B}_1$ onto the domain state $\mathbf{B}_k$. The elements of the space group $\mathcal{H}_1$ map the domain state of $\mathbf{B}_1$ onto itself: $h_m\mathbf{B}_1 = \mathbf{B}_1$, $h_m \in \mathcal{H}_1$. Therefore, not just the element g_k but all elements $g_k h_m$ of the coset $g_k\mathcal{H}_1$ map the domain state of $\mathbf{B}_1$ onto the domain state $\mathbf{B}_k$: $\mathbf{B}_k = g_k\mathcal{H}_1\mathbf{B}_1 = g_k\mathbf{B}_1$. This can be expressed in the form:

There is a one-to-one correspondence between the cosets of the decomposition $(\mathcal{G} : \mathcal{H}_1)$ and the possible domain states which may be observed after the transition.

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[11] A phase transition is called non-ferroelastic if the space groups $\mathcal{G}$ and $\mathcal{H}$ belong to the same crystal family, of which there are six: triclinic, monoclinic, orthorhombic, tetragonal, trigonal–hexagonal and cubic. A phase transition is called ferroelastic if the strain tensor of the low-symmetry phase **B** has more independent components than the strain tensor of the high-symmetry phase **A**. This can only happen if the space groups $\mathcal{G}$ of **A** and $\mathcal{H}$ of **B** belong to different crystal families. In this case, the additional components of the strain tensor of **B** are called *spontaneous strain-tensor components* or *components of the spontaneous deformation.*

references