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onto a domain state $\mathbf{B}_j$ with another directional state which results in the following lemma:

Lemma 1.2.7.2.7. The number of directional states in the transition $\mathbf{A} \longrightarrow \mathbf{B}$ with space groups $\mathcal{G}$ and $\mathcal{H}_1$ is $|\mathcal{G} : \mathcal{M}_1|$, *i.e.* the index $[i_P]$ of $\mathcal{M}_1$ in $\mathcal{G}$. □

The number of directional states does not depend on the type of description, whether microscopic or continuum, and is thus the same for both. Therefore, the microscopic description of the directional state may form a bridge between both kinds of description.

1.2.7.3. Examples

The terms just defined shall be explained in a few examples. In Example 1.2.7.3.1 a *translationengleiche* transition is considered; *i.e.* $\mathcal{H}$ is a *translationengleiche* subgroup of $\mathcal{G}$. Because $\mathcal{M}_j = \mathcal{H}_j$, the relation between $\mathcal{G}$ and $\mathcal{H}_j$ is reflected by the relation between the space groups $\mathcal{G}$ and $\mathcal{M}_j$ and the results of the microscopic and continuum description correspond to each other.

Example 1.2.7.3.1

Perovskite $BaTiO_3$ exhibits a ferroelastic and ferroelectric phase transition from phase **A** with the cubic space group $\mathcal{G} = Pm\overline{3}m$, No. 221, to phase **B** with tetragonal space groups of type $\mathcal{H} = P4mm$, No. 99. Several aspects of this transition are discussed in *IT* D. Let $\mathbf{B}_1$ be one of the domain states of phase **B**. Because the index $|\mathcal{G} : \mathcal{H}_1| = 6$, there are six domain states, forming three pairs of domain states which point with their tetragonal c axes along the cubic x, y and z axes of $\mathcal{G}$. Each pair consists of two antiparallel domain states of opposite polarization (ferroelectric domains), related by, for example, the symmetry plane perpendicular to the symmetry axes 4.

The six domain states also form six directional states because $\mathcal{H}_j = \mathcal{M}_j$ (antiparallel domain states belong to different directional states).

To find the space groups of the domain states, the normalizers have to be determined. For the perovskite transition, the normalizer $\mathcal{N}_{\mathcal{G}}(\mathcal{H}_1)$ can be obtained from the Euclidean normalizer $\mathcal{N}_{\mathcal{E}}$ of $P4mm$ in Table 15.2.1.4 of *IT* A, which is listed as P^14/mmm. This Euclidean normalizer has continuous translations along the z direction (indicated by the P^1 lattice part of the HM symbol) and is thus not a space group. However, all additional translations of P^14/mmm are not elements of the space group $\mathcal{G}$, and $\mathcal{N}_{\mathcal{G}}(\mathcal{H}_1) = (\mathcal{N}_{\mathcal{E}}(\mathcal{H}_1) \cap \mathcal{G}) = (P^14/mmm \cap Pm\overline{3}m) = P4/mmm$ is a subgroup of $Pm\overline{3}m$ with index 3 and with the lattice of $Pm\overline{3}m$ due to the PCA. There are thus three symmetry states, *i.e.* three subgroups of the type $P4mm$ with their fourfold axes directed along the z, x and y directions of the cubic space group $\mathcal{G}$. Two domain states (with opposite polar axes) belong to each of the three subgroups $\mathcal{H}_j$ of type $P4mm$.

In Example 1.2.7.3.1, a phase transition was discussed which involves only *translationengleiche* group–subgroup relations and, hence, only directional relations between the domain states occur. Each domain state forms its own directional state. The following two examples treat *klassengleiche* transitions, *i.e.* $\mathcal{H}$ is a *klassengleiche* subgroup of $\mathcal{G}$. Then $\mathcal{M}_j = \mathcal{G}$ and there is only one directional state: a *translational domain structure*, also called *translation twin*, is formed.

The domain states of a translational domain structure differ in the origins of their space groups because of the loss of translations of the parent phase in the phase transition.

Example 1.2.7.3.2

Let $\mathcal{G} = Fm\overline{3}m$, No. 225, with lattice parameter a and $\mathcal{H}_1 = Pm\overline{3}m$, No. 221, with the same lattice parameter a. The relation $\mathcal{H}_1 < \mathcal{G}$ is *klassengleich* of index 4 and is found between the disordered and ordered modifications of the alloy $AuCu_3$. In the disordered state, one Au and three Cu atoms occupy the positions of a cubic F lattice at random; in the ordered compound the Au atoms occupy the positions of a cubic P lattice whereas the Cu atoms occupy the centres of all faces of this cube. According to *IT* A, Table 15.2.1.4, the Euclidean normalizer of $\mathcal{H}_1$ is $\mathcal{N}_{\mathcal{E}}(\mathcal{H}_1) = Im\overline{3}m$ with lattice parameter a. The additional I-centring translations of $\mathcal{N}_{\mathcal{E}}(\mathcal{H}_1)$ are not translations of $\mathcal{G}$ and thus $\mathcal{N}_{\mathcal{G}}(\mathcal{H}_1) = \mathcal{H}_1$. There are four domain states, each one with its own distinct space group $\mathcal{H}_j$, $j = 1, \ldots, 4$, and symmetry state. The shifts of the conventional origins of $\mathbf{B}_j$ relative to the origin of **A** are 0, 0, 0; $\frac{1}{2}, \frac{1}{2}, 0$; $\frac{1}{2}, 0, \frac{1}{2}$; and $0, \frac{1}{2}, \frac{1}{2}$. These shifts do not show up in the macroscopic properties of the domains but in the mismatch at the boundaries (antiphase boundaries) where different domains (antiphase domains) meet. This may be observed, for example, by high-resolution transmission electron microscopy (HRTEM), *IT* D, Section 3.3.10.6.

In the next example there are two domain states and both belong to the same space group, *i.e.* to the same symmetry state.

Example 1.2.7.3.3

There is an order–disorder transition of the alloy β-brass, CuZn. In the disordered state the Cu and Zn atoms occupy at random the positions of a cubic I lattice with space group $\mathcal{G} = Im\overline{3}m$, No. 229. In the ordered state, both kinds of atoms form a cubic primitive lattice P each, and one kind of atom occupies the centres of the cubes of the other, as in the CsCl crystal structure. Its space group is $\mathcal{H} = Pm\overline{3}m$, No. 221, which is a subgroup of index [2] of $\mathcal{G}$ with the same cubic lattice parameter a. There are two domain states with their crystal structures shifted relative to each other by $\frac{1}{2}(\mathbf{a} + \mathbf{b} + \mathbf{c})$. The space group $\mathcal{H}$ is a normal subgroup of $\mathcal{G}$ and both domain states belong to the same symmetry state.

Up to now, only examples with *translationengleiche* or *klassengleiche* transitions have been considered. Now we turn to the domain structure of a *general* transition, where $\mathcal{H}$ is a general subgroup of $\mathcal{G}$. General subgroups are never maximal subgroups and are thus not listed in this volume, but have to be derived from the maximal subgroups of each single step of the group–subgroup chain between $\mathcal{G}$ and $\mathcal{H}$. In the following Example 1.2.7.3.4, the chain has two steps.

Example 1.2.7.3.4

β-Gadolinium molybdate, $Gd_2(MoO_4)_3$, is ferroelectric and ferroelastic. It was treated as an example from different points of view in *IT* D by Tolédano (Section 3.1.2.5.2) and by Janovec & Přívratská (Example 3.4.2.6). The high-temperature phase **A** has space group $\mathcal{G} = P\overline{4}2_1m$, No. 113, and basis vectors **a**, **b** and **c**. A phase transition to a low-temperature phase **B** occurs with space-group type $\mathcal{H} = Pba2$, No. 32, basis vectors $\mathbf{a}' = \mathbf{a} - \mathbf{b}$, $\mathbf{b}' = \mathbf{a} + \mathbf{b}$ and $\mathbf{c}' = \mathbf{c}$. In addition to the reduction of the point-group symmetry the primitive unit cell is doubled. The PCA will be applied because the transition from the tetragonal to the orthorhombic crystal family would without the PCA allow $a' \neq b'$ for the lattice parameters. The index of $\mathcal{H}$ in $\mathcal{G}$ is $[i] = |P\overline{4}2_1m : Pba2| = 4$ such that there are four domain states. These relations are displayed in Fig. 1.2.7.1.

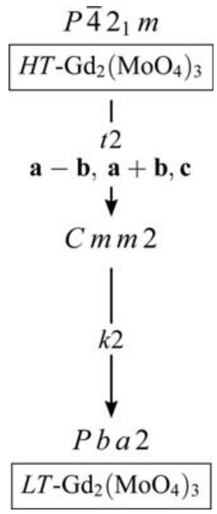

Fig. 1.2.7.1. Group–subgroup relations between the high (*HT*) and low temperature (*LT*) forms of gadolinium molybdate (Bärnighausen tree as explained in Section 1.6.3).

To calculate the number of space groups *Pba*2, *i.e.* the number of symmetry states, one determines the normalizer of *Pba*2 in $P\bar{4}2_1m$. From *IT* A, Table 15.2.1.3, one finds $\mathcal{N}_{\mathcal{E}}(Pba2) = P^1 4/mmm$ for the Euclidean normalizer of *Pba*2 under the PCA, which includes the condition $a' = b'$. $P^1 4/mmm$ is a supergroup of $P\bar{4}2_1m$. Thus, $\mathcal{N}_{\mathcal{G}}(Pba2) = (\mathcal{N}_{\mathcal{E}}(Pba2) \cap \mathcal{G}) = \mathcal{G}$ and *Pba*2 is a normal subgroup. Therefore, under the PCA all four domain states belong to one space group *Pba*2, *i.e.* there is one symmetry state. Indeed, the tables of Volume A1 list only one subgroup of type *Cmm*2 under $P\bar{4}2_1m$ and only one subgroup *Pba*2 under *Cmm*2 with $[i] = 2$ in both cases. Hermann's group $\mathcal{M}$, $\mathcal{G} > \mathcal{M} > \mathcal{H}$ is of space-group type *Cmm*2 with the point group *mm*2 of $\mathcal{H}$ and with the lattice of $\mathcal{G}$. Because $|\mathcal{G} : \mathcal{M}| = 2$, there are two directional states which belong to the same space group. The directional state of $\mathbf{B}_2$ is obtained from that of $\mathbf{B}_1$ by, for example, the (lost) $\bar{4}$ operation of $P\bar{4}2_1m$: the basis vector **a** of $\mathbf{B}_2$ is parallel to **b** of $\mathbf{B}_1$, **b** of $\mathbf{B}_2$ is parallel to **a** of $\mathbf{B}_1$ and **c** of $\mathbf{B}_2$ is antiparallel to **c** of $\mathbf{B}_1$. The other factor of 2 is caused by the loss of the centring translations of *Cmm*2, $i_T = |\mathcal{M} : \mathcal{H}| = 2$. Therefore, the domain state $\mathbf{B}_3$ is parallel to $\mathbf{B}_1$ but its origin is shifted with respect to that of $\mathbf{B}_1$ by a lost translation, for example, by $t(1, 0, 0)$ of $\mathcal{G}$, which is $t(\frac{1}{2}, \frac{1}{2}, 0)$ in the basis $\mathbf{a}'$, $\mathbf{b}'$ of *Pba*2. The same holds for the domain state $\mathbf{B}_4$ relative to $\mathbf{B}_2$.

1.2.8. Lemmata on subgroups of space groups

There are several lemmata on subgroups $\mathcal{H} < \mathcal{G}$ of space groups $\mathcal{G}$ which may help in getting an insight into the laws governing group–subgroup relations of plane and space groups. They were also used for the derivation and the checking of the tables of Part 2. These lemmata are proved or at least stated and explained in Chapter 1.4. They are repeated here as statements, separated from their mathematical background, and are formulated for the three-dimensional space groups. They are valid by analogy for the (two-dimensional) plane groups.

1.2.8.1. General lemmata

Lemma 1.2.8.1.1. A subgroup $\mathcal{H}$ of a space group $\mathcal{G}$ is a space group again, if and only if the index $i = |\mathcal{G} : \mathcal{H}|$ is finite. □

In this volume, only subgroups of finite index *i* are listed. However, the index *i* is not restricted, *i.e.* there is no number *I* with the property $i < I$ for any *i*. Subgroups $\mathcal{H} < \mathcal{G}$ with infinite index are considered in *International Tables for Crystallography*, Volume E (2002).

Lemma 1.2.8.1.2. Hermann's theorem. For any group–subgroup chain $\mathcal{G} > \mathcal{H}$ between space groups there exists a uniquely defined space group $\mathcal{M}$ with $\mathcal{G} \geq \mathcal{M} \geq \mathcal{H}$, where $\mathcal{M}$ is a *translationengleiche* subgroup of $\mathcal{G}$ and $\mathcal{H}$ is a *klassengleiche* subgroup of $\mathcal{M}$. □

The decisive point is that any group–subgroup chain between space groups can be split into a *translationengleiche* subgroup chain between the space groups $\mathcal{G}$ and $\mathcal{M}$ and a *klassengleiche* subgroup chain between the space groups $\mathcal{M}$ and $\mathcal{H}$.

It may happen that either $\mathcal{G} = \mathcal{M}$ or $\mathcal{H} = \mathcal{M}$ holds. In particular, one of these equations must hold if $\mathcal{H} < \mathcal{G}$ is a maximal subgroup of $\mathcal{G}$.

Lemma 1.2.8.1.3. (Corollary to Hermann's theorem.) A maximal subgroup of a space group is either a *translationengleiche* subgroup or a *klassengleiche* subgroup, never a general subgroup. □

The following lemma holds for space groups but not for arbitrary groups of infinite order.

Lemma 1.2.8.1.4. For any space group, the number of subgroups with a given finite index *i* is *finite.* □

This number of subgroups can be further specified, see Chapter 1.4. Although for each index *i* the number of subgroups is finite, the number of all subgroups with finite index is infinite because there is no upper limit for the number *i*.

1.2.8.2. Lemmata on maximal subgroups

Even the set of all *maximal* subgroups of finite index is not finite, as can be seen from the following lemma.

Lemma 1.2.8.2.1. The index *i* of a maximal subgroup of a space group is always of the form p^n, where *p* is a prime number and n = 1 or 2 for plane groups and n = 1, 2 or 3 for space groups. □

This lemma means that a subgroup of, say, index 6 cannot be maximal. Moreover, because of the infinite number of primes, the set of all maximal subgroups of a given space group cannot be finite.

An index of p^2, $p > 2$, occurs for isomorphic subgroups of tetragonal space groups when the basis vectors are enlarged to $p\mathbf{a}$, $p\mathbf{b}$; for trigonal and hexagonal space groups, the enlargement $p\mathbf{a}$, $p\mathbf{b}$ is allowed for $p = 2$ and for all or part of the primes $p > 3$. An index of p^3 occurs for and only for isomorphic subgroups of cubic space groups with cell enlargements of $p\mathbf{a}$, $p\mathbf{b}$, $p\mathbf{c}$ ($p > 2$).

There are even stronger restrictions for *maximal non-isomorphic* subgroups.

Lemma 1.2.8.2.2. The index of a maximal non-isomorphic subgroup of a plane group is 2 or 3; for a space group the index is 2, 3 or 4. □

This lemma can be specified further:

Lemma 1.2.8.2.3. The index of a maximal non-isomorphic subgroup $\mathcal{H}$ is always 2 for oblique, rectangular and square plane groups and for triclinic, monoclinic, orthorhombic and tetragonal space groups $\mathcal{G}$. The index is 2 or 3 for hexagonal plane groups and for trigonal and hexagonal space groups $\mathcal{G}$. The index is 2, 3 or 4 for cubic space groups $\mathcal{G}$. □