point group. The orientation state $\mathbf{B}_2$ is obtained from $\mathbf{B}_1$ by the (lost) $\overline{4}$ operation of $\overline{4}2m$.

This is the *macroscopic* or *continuum treatment*; it is the most common treatment of domains in phase transitions. In reality, *i.e.* lifting the PCA, due to the orthorhombic symmetry of phase $\mathbf{B}$ the domains will be slightly distorted and rotated, and thus the symmetry planes of the two domain states are no longer parallel.

The full microscopic or atomistic treatment has to consider the crystal structures of phases $\mathbf{A}$ and $\mathbf{B}$. Under the PCA, the length of a' and b' is $(2)^{1/2}a$, the content of the unit cell of $\mathbf{B}_1$ is twice that of $\mathbf{A}$. Because the index $[i] = 4$ there are four domain states $\mathbf{B}_1$ to $\mathbf{B}_4$ of $Pba2$. The domain state $\mathbf{B}_2$ is obtained from $\mathbf{B}_1$ by the (lost) $\overline{4}$ operation of $P\overline{4}2_1m$. The same holds for the pair $\mathbf{B}_3$ and $\mathbf{B}_4$. Thus, $\mathbf{B}_2$ & $\mathbf{B}_4$ are rotated by $90°$ around a $\overline{4}$ centre in the $(a'\,b')$ plane with respect to the pair $\mathbf{B}_1$ & $\mathbf{B}_3$, and the c' axes are antiparallel for $\mathbf{B}_2$ & $\mathbf{B}_4$ relative to those of $\mathbf{B}_1$ & $\mathbf{B}_3$. The orientation state of the pair $\mathbf{B}_1$ & $\mathbf{B}_3$ is different from that of $\mathbf{B}_2$ & $\mathbf{B}_4$. The two pairs $\mathbf{B}_1$ & $\mathbf{B}_2$ and $\mathbf{B}_3$ & $\mathbf{B}_4$ are shifted relative to each other by a (lost) translation of $P\overline{4}2_1m$, *e.g.* by $t(1,0,0)$ in the basis of $P\overline{4}2_1m$, corresponding to $t(\frac{1}{2},\frac{1}{2},0)$ in the basis of $Pba2$.

To calculate the number of space groups $Pba2$, *i.e.* the number of symmetry states, one determines the normalizer of $Pba2$ in $P\overline{4}2_1m$. From *IT* A, Table 15.2.1.3, one finds $\mathcal{N}_{\mathcal{E}}(Pba2) = P^14/mmm$ for the Euclidean normalizer of $Pba2$ under the PCA, which includes the condition $a = b$. P^14/mmm is a supergroup of $P\overline{4}2_1m$. Thus, $\mathcal{N}_{\mathcal{G}}(Pba2) = (\mathcal{N}_{\mathcal{E}}(Pba2) \cap \mathcal{G}) = \mathcal{G}$ and $|\mathcal{G} : \mathcal{N}_{\mathcal{G}}(Pba2)| = |\mathcal{G} : \mathcal{G}| = 1$. Therefore, under the PCA all four domain states belong to one symmetry state, *i.e.* to one space group $Pba2$.

Analysing the group–subgroup relations between $P\overline{4}2_1m$ and $Pba2$ with the tables of this volume, one finds only one chain $P\overline{4}2_1m \rightarrow Cmm2 \rightarrow Pba2$. For $P\overline{4}2_1m$ only one maximal subgroup of type $Cmm2$ is listed, for which again only one maximal subgroup of type $Pba2$ is found, in agreement with the previous paragraph.

In reality, *i.e.* relaxing the PCA, the observations are made at temperatures $T_x < T_C$ where the lattice parameters deviate from those of phase $\mathbf{A}$ and the basis no longer has tetragonal symmetry, but orthorhombic symmetry, $a' < b'$. The previous single space group now splits into *two* different space groups of type $Pba2$ with orthorhombic metrics at T_x, one belonging to the pair $\mathbf{B}_1$ & $\mathbf{B}_3$, the other to $\mathbf{B}_2$ & $\mathbf{B}_4$. The $(\mathbf{a}', \mathbf{b}')$ bases of these pairs are oriented perpendicular to each other and the $\mathbf{c}'$ axes of their domains are antiparallel. The loss of the centring translation of $Cmm2$ does not produce a new space group.

The number, two, of these space groups if the PCA is not valid can also be calculated in the usual way with the help of the normalizer. The Euclidean normalizer of $Pba2$ with $a' \neq b'$ is $\mathcal{N}_{\mathcal{E}}(Pba2) = P^1mmm$. This is an orthorhombic group with continuous translations along the $\mathbf{c}'$ direction. P^1mmm with $a' \neq b'$ is not really a subgroup of $P\overline{4}2_1m$ because the translations of $Pba2$ and thus of $Cmm2$ and P^1mmm are not strictly translations of $P\overline{4}2_1m$. The first three groups have orthorhombic lattices and the last a tetragonal one. However, by relaxing the PCA only gradually, the difference between the orthorhombic groups and the corresponding groups with tetragonal lattices is arbitrarily small. Therefore, one considers the sequence $\mathcal{G} > \mathcal{M} = \mathcal{N}_{\mathcal{G}}(\mathcal{H}) > \mathcal{H}$, *i.e.* $P\overline{4}2_1m > Cmm2 > Pba2$ as a group–subgroup chain, forms the intersection $(P^1mmm \cap P\overline{4}2_1m)$ as if the groups would have common translations, and finds $\mathcal{N}_{\mathcal{G}}(\mathcal{H}) = Cmm2$ with approxi-

mately the lattice parameters of $P\overline{4}2_1m$. The index $|P\overline{4}2_1m : Cmm2| = 2$, such that there are two space groups of type $Pba2$ which are approximately subgroups of $P\overline{4}2_1m$. To each of these space groups $Pba2$ belong two domain states of phase $\mathbf{B}$, see above.

This example shows that without the PCA, in order to cope with real observations, the terms 'subgroup', 'intersection of groups' *etc.* must not be used *sensu stricto* but have to be relaxed. The orthorhombic translations in this example are not group elements of $\mathcal{G}$ but are slightly modified from the original translations of $\mathcal{G}$. All group–subgroup relations in crystal chemistry, *e.g.* diamond (C)–sphalerite (ZnS), as well as many phase transitions, as in this example, require such a 'softened' approach.

It turns out that the transition of $Gd_2(MoO_4)_3$ can be considered both under the PCA (allowing exact group-theoretical arguments) and under physically realistic arguments (which require certain relaxations of the group-theoretical methods). The results are different but the realistic approach can be developed by means of an increasing deviation from the PCA, starting from idealized but unrealistic considerations.

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 1.5. 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*, Vol. 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 1.5. 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. □

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

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.

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 $\mathcal{G}$. □

There are also lemmata for the number of subgroups of a certain index. The most important are:

Lemma 1.2.8.2.4. The number of subgroups of index 2 is $2^N - 1$ with $0 \leq N \leq 6$ for space groups and $0 \leq N \leq 4$ for plane groups. The number of *translationengleiche* subgroups of index 2 is $2^M - 1$ with $0 \leq M \leq 3$ for space groups and $0 \leq M \leq 2$ for plane groups. □

Examples are:
$N = 0$: $2^0 - 1 = 0$ subgroups of index 2 for $p3$, No. 13, and $F23$, No. 196;
$N = 1$: $2^1 - 1 = 1$ subgroup of index 2 for $p3m1$, No. 14, and $P3$, No. 143; ... ;
$N = 4$: $2^4 - 1 = 15$ subgroups of index 2 for $p2mm$, No. 6, and $P\bar{1}$, No. 2;
$N = 6$: $2^6 - 1 = 63$ subgroups of index 2 for *Pmmm*, No. 47.

Lemma 1.2.8.2.5. The number of isomorphic subgroups of each space group is infinite and this applies even to the number of maximal isomorphic subgroups. □

Nevertheless, their listing is possible in the form of infinite series. The series are specified by parameters.

Lemma 1.2.8.2.6. For each space group, each maximal isomorphic subgroup $\mathcal{H}$ can be listed as a member of one of at most four series of maximal isomorphic subgroups. Each member is specified by a set of parameters. □

The series of maximal isomorphic subgroups are discussed in Section 2.1.5.