(iv) *Additional remark*. The pseudo-hexagonal triple growth twins are morphologically often described by a pseudo-threefold rotation with angle $\phi' = 2\arctan(b/a)$, clockwise ($\phi'+$) for domain pair $1 \rightarrow 2$ and anticlockwise ($\phi'-$) for domain pair $1 \rightarrow 3$, both together approximately filling the full 360° circle. The basis-vector transformations (1) and (2) given above for $m'(110)$ and $m'(1\bar{1}0)$ have to be modified as follows: The vectors $\mathbf{a}_2$ and $\mathbf{a}_3$ remain unchanged, whereas $\mathbf{b}_2$ and $\mathbf{b}_3$ are inverted into their opposites $-\mathbf{b}_2$ and $-\mathbf{b}_3$, thus leading to right-handed coordinate systems for domains 2 and 3. Similarly for h_2, k_2, h_3 and k_3 [equations (3) and (4) above]. Since the reversal of the axis **b** is part of the *eigensymmetry* of point group *mmm*, the effect of $\phi'+$ and $\phi'-$ is the same as that of $m'(110)$ and $m'(1\bar{1}0)$. Thus each of the three twin elements $m'(110)$, $2'_{\rm irrat} \simeq [310]$ and $\phi'+$ represents in point group *mmm* the same orientation relation for domain pair $1 \rightarrow 2$. Similarly: $m'(1\bar{1}0)$, $2'_{\rm irrat} \simeq [3\bar{1}0]$ and $\phi'-$ for domain pair $1 \rightarrow 3$.

For the hemihedral point groups 222 and *mm*2, *m*2*m*, 2*mm* these results have to be modified. For group 222 the two reflection twin elements lead to opposite handedness of domains 1 and 2 and 1 and 3, but equal handedness of domains 2 and 3, whereas twin elements $2'_{\rm irrat}$ and $\phi'\pm$ provide equal handedness of all three domains. For point group *mm*2 *etc.* the situation is more complicated due to the different settings with the polar axis along **a**, **b** or **c**, which physically lead to polar domains with different head-to-tail, head-to-head and tail-to-tail domain boundaries. These cases are not further analysed here.

Concerning the diffraction patterns of pseudo-hexagonal twins of hemihedral orthorhombic crystals: The splitting of diffraction spots is a matter of the lattice metric and independent of the point group. Regarding reflection intensities: among the triply split reflections only reflections of sets {*hhl*} and {*h*,3*h*,*l*} may undergo a change from diffraction case A in point groups *mmm* to diffraction case B2 in the hemihedral groups.

3.3.11.6. *Programs for structure determinations with twinned crystals*

Programs for the determination of crystal structures from merohedral and pseudo-merohedral twins are, among others, *SFLS* (Eitel & Bärnighausen, 1986), *TWINXLI* (Hahn & Massa, 1997), *TWIN* 3.0 (Kahlenberg & Messner, 2001), *CRYSTALS* 12 (Betteridge *et al*., 2003), *JANA*2006 (Petricek *et al*., 2006), *DIRAX* (A. J. M. Van Duisenberg, University of Utrecht, The Netherlands; e-mail: duisenberg@chem.uu.nl) and especially *SHELXL* (Sheldrick, 1997).

Detailed descriptions of the (widely used) *SHELXL* program system for structure determinations and for refinements of merohedrally and pseudo-merohedrally twinned crystals are provided by Herbst-Irmer & Sheldrick (1998, 2002), by Guzei *et al*. (2012) and, in particular, by Herbst-Irmer (2006).

Textbook descriptions of structure determinations of twins are provided by Buerger (1960*a*), Massa (2004) and Ferraris (2004). Systematic analyses of the diffraction intensities of all Σ1, Σ3, Σ5 and Σ7 merohedral twins are contained in two publications by Klapper & Hahn (2010, 2012).

The following note on domain structures is supplied by V. Janovec. It describes briefly and clearly how strategies used in the study of 'domain structures', treated in Chapter 3.4, can be used for the investigation of twins. Section 3.3.12 thus forms a bridge between the present chapter on *Twinning* and the following chapter on *Domain structures*.

3.3.12. Domain structures (by V. Janovec)

Domain structure is a special kind of twinning which *results from lowering of crystal symmetry* at a phase transition. A homogeneous phase with higher symmetry (called the *parent phase*) breaks into a non-homogeneous twinned phase (ferroic phase) with lower symmetry in which the twin partners (*domains*) are related by twinning operations that are crystallographic operations disappearing at the transition (for different terminology used in twinning and domain structures, see Table 3.4.2.4).

Domains have lower symmetry than the parent phase. As a result, domains acquire additional physical properties called *spontaneous properties*. When observed by certain apparatus (*e.g.* a microscope), anisotropic domains exhibit different properties and thus can be observed and identified in direct space. This distinction of domains in direct space by means of their spontaneous properties thus provides important additional information to the examination of twinning of the material by diffraction methods.

It turns out that symmetry lowering at the transition exactly determines which spontaneous quantities are distinct in the two different domains of a domain twin. Unfortunately, this useful consideration cannot be performed with twins which originate from means other than a phase transition, *e.g.* growth twins. It is, however, possible to check whether the nonexistent high-symmetry parent phase can be substituted by a so-called *composite symmetry* of the twin, even though a phase of the crystal with this symmetry does not exist in reality. This means that we *treat a twin as a domain twin resulting from a nonexistent (hypothetical) phase transition*.

This is why it is expedient to have at one's disposal tables of possible phase transitions from all possible composite symmetries. These tables can be found in Sections 3.4.3 and 3.4.4 of Chapter 3.4. Several examples show how these tables can be utilized in twin analysis.

3.3.13. Glossary

(hkl)	crystal face, lattice plane, net plane (Miller indices)
$\{hkl\}$	crystal form, set of symmetry-equivalent lattice (net) planes
$[uvw]$	zone axis, crystal edge, lattice direction, lattice row (direction indices)
$\langle uvw \rangle$	set of symmetry-equivalent lattice directions (rows)
$\mathcal{G}$	symmetry group of the (real or hypothetical) 'parent structure' or high-symmetry modification or 'prototype phase' of a crystal; group in general
$\mathcal{H}$	*eigensymmetry* group of an (untwinned) crystal; symmetry group of the deformed ('daughter') phase of a crystal; subgroup
$\mathcal{H}_1, \mathcal{H}_2, \ldots, \mathcal{H}_j$	oriented *eigensymmetries* of domain states 1, 2, …, *j*
$\mathcal{H}^*_{1,2}, \mathcal{H}^*$	intersection symmetry group of the pair of oriented *eigensymmetries* $\mathcal{H}_1$ and $\mathcal{H}_2$, reduced *eigensymmetry* of a domain
$\mathcal{K}$	composite symmetry group of a twinned crystal (domain pair); twin symmetry
$\mathcal{K}^*_{1,2}, \mathcal{K}^*$	reduced composite symmetry of the domain pair (1, 2)
$\mathcal{K}(n)$	extended composite symmetry of a twinned crystal with a pseudo *n*-fold twin axis
$k, k_1, k_2, \ldots, k_i$	twin operations (k_1 = identity)
$2', m', \bar{1}', 4'(2), \underline{6}'(3), \bar{3}'(3), \bar{6}'(3)$	twin operations of order two in colour-changing (black–white) symmetry notation
$\lvert\mathcal{G}\rvert, \lvert\mathcal{H}\rvert, \lvert\mathcal{K}\rvert$	order of group $\mathcal{G}$, $\mathcal{H}$, $\mathcal{K}$
$[i]$	index of $\mathcal{H}$ in $\mathcal{G}$, or of $\mathcal{H}$ in $\mathcal{K}$
$[j]$, Σ	index of coincidence-site lattice (twin lattice, sublattice) with respect to crystal lattice

ω	twin obliquity
$\mathbf{b}_t$	Burgers vector of twinning dislocations
$\mathbf{f}$	fault vector of a merohedral twin boundary
$\mathbf{t}$	twin displacement vector
$\mathcal{G}F\mathcal{H}$ or $\mathcal{G} > F$	Aizu (1970*a*) symbol of a ferroic phase transition (ferroic species); F = ferroic
W, W'	designation of non-merohedral ferroelastic twin boundaries (according to Sapriel, 1975)
F_{hkl}	structure factor of reflection hkl
$\mathbf{g}_{hkl}$	diffraction vector (reciprocal-lattice vector) of reflection hkl
φ_{hkl}	phase angle of structure factor F_{hkl}
Ψ_{hkl}, Φ_{hkl}	difference of phase angles ('phase jump') across twin boundary
ρ	charge density of a ferroelectric twin boundary
$\mathbf{P}$	spontaneous polarization

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