(i) For *twin interfaces*, only the terms *coherent* and *incoherent* are used. In view of the fact that twin interfaces do not require regular (perfect) dislocations (but may contain twinning dislocations as described above in Section 3.3.10.8), the term 'semi-coherent' is reserved for grain boundaries and heterophase interfaces.

(ii) Twin boundaries are called *coherent* only if they are (mechanically) compatible. This holds for both rational and irrational twin boundaries, as suggested by Christian (1965, p. 332). Both cases may be distinguished by using qualifying adjectives such as 'rationally coherent' and 'irrationally coherent'. Note that irrational (compatible) twin boundaries are usually less perfect and of higher energy than rational ones.

(iii) For strict merohedral (non-ferroelastic) twins (lattice index $[j] = 1$) any twin boundary, even a curved one, is compatible and, hence, is designated here as *coherent*, even if the contact plane does not coincide with the twin mirror plane.

(iv) For non-merohedral (ferroelastic) twins, a pair of (rational or irrational) perpendicular compatible interfaces occurs (Section 3.3.10.2.1). The same holds for merohedral twins of lattice index $[j] > 1$ (Section 3.3.10.2.4). All these compatible boundaries are considered here as *coherent*.

(v) In lattice and structural terms, a twin boundary is *coherent* if it exhibits a well defined matching of the two lattices along the entire boundary, *i.e.* continuity with respect to their lattice vectors and lattice planes. We want to stress that we consider the coherence of a twin boundary not as being destroyed by the presence of a nonzero twin displacement or fault vector as long as there is an optimal low-energy fit of the two partner structures. The twin displacement (fault) vector represents a 'phase shift' between the two structures with the same two-dimensional periodicity along their contact plane and thus defines the continuity relation across the boundary. This statement agrees with the general opinion that stacking faults, antiphase boundaries and many merohedral twin boundaries, all possessing nonzero fault vectors, are *coherent*. Well known examples are stacking faults in f.c.c and h.c.p metals and Brazil twin boundaries in quartz.

It is apparent from these discussions of *coherent* twin interfaces that several features have to be taken into account, some readily available by experiments and observations, whereas others require geometric models (lattice matching) or even physical models (structure matching), including determination of twin displacement vectors **t**.

The definitions of *coherence*, as treated here, often do not satisfactorily agree with reality. Two examples are given:

(*a*) Japanese twins of quartz with twin mirror plane $(11\bar{2}2)$ or twofold twin axis normal to $(11\bar{2}2)$. According to the definitions given above, the observed $(11\bar{2}2)$ contact plane is *coherent*. Nevertheless, these $(11\bar{2}2)$ boundaries are always strongly disturbed and accompanied by extended lattice distortions. Thus, in reality they must be considered as *not coherent*.

(*b*) Sodium lithium sulfate, $NaLiSO_4$, with polar point group $3m$ and a hexagonal lattice forms merohedral growth twins with twin mirror plane (0001) normal to the polar axis. The composition plane coincides with the twin plane and has head-to-head or tail-to-tail character. According to definition (iii) above, any twin boundary of this merohedral twin is *coherent*. The observed (0001) contact plane, however, despite coincidence with the twin mirror plane, is always strongly disturbed and cannot be considered as coherent. In this case, the observed *incoherence* is obviously due to the head-to-head orientation of the boundary, which is 'electrically forbidden'.

These examples demonstrate that the above formal definitions of *coherence*, based on geometrical viewpoints alone, are not always satisfactory and require consideration of individual cases.

With these discussions of rather subtle features of twin interfaces, this chapter on twinning is concluded. It was our aim to present this rather ancient topic in a way that progresses from classical concepts to modern considerations, from three dimensions to two and from macroscopic geometrical arguments to microscopic atomistic reasoning. Macroscopic derivations of orientation and contact relations of the twin partners (twin laws, as well as twin morphologies and twin genesis) were followed by lattice considerations and structural implications of twinning. Finally, the physical background of twinning was explored by means of the analysis of twin interfaces, their structural and energetic features. It is this latter aspect which in the future is most likely to bring the greatest progress toward the two main goals, an atomistic understanding of the phenomenon 'twinning' and the ability to predict correctly its occurrence and non-occurrence.

All considerations in this chapter refer to analysis of twinning in *direct space*. The complementary aspect, the effect of twinning in *reciprocal space*, lies beyond the scope of the present treatment and, hence, had to be omitted. This concerns in particular the recognition and characterization of twinning in diffraction experiments, especially by X-rays, as well as the consideration of the problems that twinning, especially merohedral twinning, may pose in single-crystal structure determination (*cf.* Buerger, 1960*a*). Several powerful computer programs for the solution of these problems exist. For a case study, see Herbst-Irmer & Sheldrick (1998).

3.3.11. Glossary

(hkl)	crystal face, lattice plane, net plane (Miller indices)
$\{hkl\}$	crystal form, set of symmetrically equivalent lattice (net) planes
$[uvw]$	zone axis, crystal edge, lattice direction, lattice row (direction indices)
$\langle uvw \rangle$	set of symmetrically 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 $1, 2, \ldots, j$
$\mathcal{H}^*_{1,2}, \mathcal{H}^*$	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
f	fault vector of a merohedral twin boundary
t	twin displacement vector

$\mathcal{GFH}$	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
P	spontaneous polarization

We are indebted to Elke Haque (Bonn), Zdenek Janovec (Prague) and Stefan Klumpp (Bonn) for preparing the figures. We are grateful to Vaclav Janovec (Prague) for fruitful discussions and to our editor André Authier for his patience and help in preparing the manuscript.

References

Abrahams, S. C. (1994). *Structure relationship to dielectric, elastic and chiral properties. Acta Cryst.* A**50**, 658–685.

Aizu, K. (1969). *Possible species of 'ferroelastic' crystals and of simultaneously ferroelectric and ferroelastic crystals. J. Phys. Soc. Jpn*, **27**, 387–396.

Aizu, K. (1970*a*). *Possible species of ferromagnetic, ferroelectric and ferroelastic crystals. Phys. Rev. B*, **2**, 754–772.

Aizu, K. (1970*b*). *Determination of the state parameters and formulation of spontaneous strain for ferroelastics. J. Phys. Soc. Jpn*, **28**, 706–716.

Aizu, K. (1973). *Second-order ferroic state shifts. J. Phys. Soc. Jpn*, **34**, 121–128.

Amelinckx, S., Gevers, R. & Van Landuyt, J. (1978). Editors. *Diffraction and imaging techniques in materials science*, Vol. I. *Electron microscopy*, especially pp. 107–151. Amsterdam: North-Holland.

Aminoff, G. & Broomé, B. (1931). *Strukturtheoretische Studien über Zwillinge I. Z. Kristallogr.* **80**, 355–376.

Arlt, G. (1990). *Twinning in ferroelectric and ferroelastic ceramics: stress relief. J. Mater. Sci.* **25**, 2655–2666.

Arzruni, A. (1887). *Ein neues Zwillingsgesetz im regulären System. Proc. Russ. Mineral. Soc. St. Petersburg*, **23**, 126–132. (In German.)

Authier, A. & Sauvage, M. (1966). *Dislocations de macle dans la calcite: interférences entre les champs d'onde créés à la traversée d'une lamelle de macle. J. Phys. Rad. (France)*, **27**, 137–142.

Barber, D. J. & Wenk, H.-R. (1979). *Deformation twinning in calcite, dolomite, and other rhombohedral carbonates. Phys. Chem. Miner.* **5**, 141–165.

Barrett, C. S. & Massalski, T. B. (1966). *Structure of metals*, 3rd edition, especially pp. 406–414. New York: McGraw-Hill.

Bartels, H. & Follner, H. (1989). *Crystal growth and twin formation of gypsum. Cryst. Res. Technol.* **24**, 1191–1196.

Baumhauer, H. (1879). *Über künstliche Kalkspath-Zwillinge nach -1/2R. Z. Kristallogr.* **3**, 588–591.

Becke, F. (1911). *Über die Ausbildung der Zwillingskristalle. Fortschr. Mineral. Kristallogr. Petrogr.* **1**, 48–65.

Billiet, Y. & Bertaut, E. F. (2002). *Isomorphic subgroups of space groups.* Part 13 of *International tables for crystallography*, Vol. A. *Space-group symmetry*, edited by Th. Hahn, 5th ed. Dordrecht: Kluwer Academic Publishers.

Bismayer, U., Röwer, R. W. & Wruck, B. (1995). *Ferroelastic phase transition and renormalization effect in diluted lead phosphate, $(Pb_{1-x}Sr_x)_3(PO_4)_2$ and $(Pb_{1-x}Ba_x)_3(PO_4)_2$. Phase Transit.* **55**, 169–179.

Black, P. J. (1955). *The structure of $FeAl_3$. II. Acta Cryst.* **8**, 175–182.

Blackburn, J. & Salje, E. K. H. (1999). *Time evolution of twin domains in cordierite: a computer simulation study. Phys. Chem. Miner.* **26**, 275–296.

Bloss, F. D. (1971). *Crystallography and crystal chemistry*, pp. 324–338. New York: Holt, Rinehart & Winston.

Bögels, G., Buijnsters, J. G., Verhaegen, S. A. C., Meekes, H., Bennema, P. & Bollen, D. (1999). *Morphology and growth mechanism of multiply twinned AgBr and AgCl needle crystals. J. Cryst. Growth*, **203**, 554–563.

Bögels, G., Meekes, H., Bennema, P. & Bollen, D. (1998). *The role of {100} side faces for lateral growth of tabular silver bromide crystals. J. Cryst. Growth*, **191**, 446–454.

Bögels, G., Pot, T. M., Meekes, H., Bennema, P. & Bollen, D. (1997). *Side-face structure and growth mechanism of tabular silver bromide crystals. Acta Cryst.* A**53**, 84–94.

Bollmann, W. (1970). *Crystal defects and crystalline interfaces.* ch. 12, pp. 143–148. Berlin: Springer.

Bollmann, W. (1982). *Crystal lattices, interfaces, matrices*, pp. 111–249. Geneva: published by the author.

Bonner, W. A. (1981). *InP synthesis and LEC growth of twin-free crystals. J. Cryst. Growth*, **54**, 21–31.

Böttcher, P., Doert, Th., Arnold, H. & Tamazyan, R. (2000). *Contributions to the crystal chemistry of rare-earth chalcogenides. I. The compounds with layer structures LnX_2. Z. Kristallogr.* **215**, 246–253.

Boulesteix, C. (1984). *A survey of domains and domain walls generated by crystallographic phase transitions causing a change of the lattice. Phys. Status Solidi A*, **86**, 11–42.

Boulesteix, C., Yangui, B., Ben Salem, M., Manolakis, C. & Amelinckx, S. (1986). *The orientation relations of interfaces between a prototype phase and its ferroelastic derivatives: theoretical and experimental studies. J. Phys.* **47**, 461–471.

Bragg, W. L. (1924). *The structure of aragonite. Proc. R. Soc. London Ser. A*, **105**, 16–39.

Bragg, W. L. (1937). *Atomic structure of minerals.* Ithaca, NY: Cornell University Press.

Bragg, W. L. & Claringbull, G. F. (1965). *The crystalline state*, Vol. IV. *Crystal structures of minerals*, p. 302. London: Bell & Sons.

Bringhurst, K. N. & Griffin, D. T. (1986). *Staurolite–lukasite series. II. Crystal structure and optical properites of a cobaltoan staurolite. Am. Mineral.* **71**, 1466–1472.

Brögger, W. C. (1890). *Hydrargillit. Z. Kristallogr.* **16**, second part, pp. 16–43, especially pp. 24–43 and Plate 1.

Bueble, S., Knorr, K., Brecht, E. & Schmahl, W. W. (1998). *Influence of the ferroelastic twin domain structure on the 100 surface morphology of $LaAlO_3$ HTSC substrates. Surface Sci.* **400**, 345–355.

Bueble, S. & Schmahl, W. W. (1999). *Mechanical twinning in calcite considered with the concept of ferroelasticity. Phys. Chem. Miner.* **26**, 668–672.

Buerger, M. J. (1934). *The lineage structure of crystals. Z. Kristallogr.* **89**, 195–220.

Buerger, M. J. (1945). *The genesis of twin crystals. Am. Mineral.* **30**, 469–482.

Buerger, M. J. (1960*a*). *Crystal-structure analyses*, especially ch. 3. New York: Wiley.

Buerger, M. J. (1960*b*). *Introductory remarks. Twinning with special regard to coherence.* In *Symposium on twinning. Cursillos y Conferencias*, Fasc. VII, pp. 3 and 5–7. Madrid: CSIC.

Buseck, P. R., Cowley, J. M. & Eyring, L. (1992). Editors. *High-resolution transmission electron microscopy and associated techniques*, especially ch. 11. New York: Oxford University Press.

Cahn, R. W. (1954). *Twinned crystals. Adv. Phys.* **3**, 202–445.

Chalmers, B. (1959). *Physical metallurgy*, especially ch. 4.4. New York: Wiley.

Chernysheva, M. A. (1950). *Mechanical twinning in crystals of Rochelle salt. Dokl. Akad. Nauk SSSR*, **74**, 247–249. (In Russian.)

Chernysheva, M. A. (1951). *Effects of an electric field on the twinned structure of Rochelle salt. Dokl. Akad. Nauk SSSR*, **81**, 1965–1968. (In Russian.)

Chernysheva, M. A. (1955). *Twinning phenomena in crystals of Rochelle salt*. PhD thesis, Moscow. (In Russian.)

Christian, J. W. (1965). *The theory of transformations in metals and alloys*, especially chs. 8 and 20. Oxford: Pergamon.

Chung, H., Dudley, M., Larson, D. J., Hurle, D. T. J., Bliss, D. F. & Prasad, V. (1998). *The mechanism of growth-twin formation in zincblende crystals: insights from a study of magnetic-liquid encapsulated Czochralski grown InP single crystals. J. Cryst. Growth,* **187**, 9–17.

Cottrell, A. H. (1955). *Theoretical structural metallurgy*, 2nd edition, especially ch. 14.5. London: Edward Arnold.

Curien, H. (1960). *Sur les axes de macle d'ordre supérieur à deux.* In *Symposium on twinning. Cursillos y Conferencias*, Fasc. VII, pp. 9–11. Madrid: CSIC.