see Section 3.3.8.2 below. These concepts were further developed by Niggli (1919, 1920/1924/1941).

The lattice aspects of twinning (*triperiodic twins*) are discussed in this section and in Section 3.3.9. An important concept in this field is the *coincidence-site sublattice* of the twin in direct space and its counterpart in reciprocal space. Extensive use of the notion of coincidence-site lattices (CSLs) is made in *bicrystallography* for the study of grain boundaries, as briefly explained in Section 3.2.2.

The coincidence-site lattice and further related lattices (O- and DSC-lattices) were introduced into the study of bicrystals by Bollmann (1970, 1982) and were theoretically thoroughly developed by Grimmer (1989, 2003). Their applications to grain boundaries are contained in the works by Sutton & Balluffi (1995) and Gottstein & Shvindlerman (1999).

3.3.8.1. *Basic concepts of Friedel's lattice theory*

The basis of Friedel's (1904, 1926) lattice theory of twinning is the postulate that the coincidence-site sublattice common to the two twin partners (twin lattice) suffers no deviation (strict condition) or at most a slight deviation (approximate condition) in crossing the boundary between the two twin components (composition plane). This purely geometrical condition is often expressed as 'three-dimensional lattice control' (Santoro, 1974, p. 225), which is supposed to be favourable to the formation of twins.

In order to define the coincidence sublattice (twin lattice) of the two twin partners, it is assumed that their oriented point lattices are infinitely extended and interpenetrate each other. The lattice classification of twins is based on the degree of coincidence of these two lattices. The criterion applied is the dimension of the *coincidence-site subset* of the two interpenetrating lattices, which is defined as the set of all lattice points common to both lattices, provided that two initial points, one from each lattice, are brought to coincidence (common origin). This common origin has the immediate consequence that the concept of the twin displacement vector **t** – as introduced in Note (8) of Section 3.3.2.4 – does not apply here. The existence of the coincidence subset of a twin results from the *crystallographic orientation relation* (Section 3.3.2.2), which is a prerequisite for twinning. This subset is one-, two- or three-dimensional (monoperiodic, diperiodic or triperiodic) twins.

If a coincidence relation exists between lattices in direct space, a complementary superposition relation occurs for their reciprocal lattices. This superposition can often, but not always, be detected in the diffraction patterns of twinned crystals.

3.3.8.2. *Lattice coincidences, twin lattice, twin lattice index*

Four types of (exact) *lattice coincidences* have to be distinguished in twinning:

(i) *No coincidence* of lattice points (except, of course, for the initial pair). This case corresponds to arbitrary intergrowth of two crystals or to a general bicrystal.

(ii) *One-dimensional coincidence*: Both lattices have only *one lattice row* in common. Of the seven binary twin operations listed in Section 3.3.2.3.1, the following three generate one-dimensional lattice coincidence:

(*a*) twofold rotation around a (rational) lattice row [twin operation (iii) in Section 3.3.2.3.1];

(*b*) reflection across an irrational plane normal to a (rational) lattice row (note that the coincidence would be three-dimensional if this plane were rational) [twin operation (iv)];

(*c*) twofold rotation around an irrational axis normal to a (rational) lattice row (complex twin, *Kantennormalengesetz*) [twin operations (v) and (vi)].

Lattices are always centrosymmetric; hence, for lattices, as well as for centrosymmetric crystals, the first two twin operations above belong to the same twin law. For noncentrosymmetric crystals, however, the two twin operations define different twin laws.

(iii) *Two-dimensional coincidence*: Both lattices have only *one lattice plane* in common. The following two (of the seven) twin operations lead to two-dimensional lattice coincidence:

(*a*) reflection across a (rational) lattice plane [twin operation (i)];

(*b*) twofold rotation around an irrational axis normal to a (rational) lattice plane (note that the coincidence would be three-dimensional if this axis were rational) [twin operation (ii)].

Again, for lattices and centrosymmetric crystals both twin operations belong to the same twin law.

(iv) *Three-dimensional coincidence*: Here the coincidence subset is a three-dimensional lattice, the *coincidence-site lattice* or *twin lattice*. It is the three-dimensional sublattice common to the (equally or differently) oriented lattices of the two twin partners. The degree of three-dimensional lattice coincidence is defined by the *coincidence-site lattice index*, *twin lattice index* or *sublattice index* [j], for short: *lattice index*. This index is often called Σ, especially in metallurgy. It is the volume ratio of the primitive cells of the twin lattice and of the (original) crystal lattice (*i.e.* $1/j$ is the 'degree of dilution' of the twin lattice with respect to the crystal lattice):

$$[j] = \Sigma = V_{\rm twin}/V_{\rm crystal}.$$

The lattice index is always an integer: $j = 1$ means *complete* coincidence (parallelism), $j > 1$ *partial* coincidence of the two lattices. The index [j] can also be interpreted as elimination of the fraction $(j-1)/j$ of the lattice points, or as index of the translation group of the twin lattice in the translation group of the crystal lattice. The coincidence lattice, thus, is the intersection of the oriented lattices of the two twin partners.

Twinning with $[j] = 1$ has been called by Friedel (1926, p. 427) *twinning by merohedry* ('*macles par mériédrie*') (for short: *merohedral twinning*), whereas twinning with $[j] > 1$ is called *twinning by lattice merohedry* or *twinning by reticular merohedry* ('*macles par mériédrie réticulaire*') (Friedel, 1926, p. 444). The terms for $[j] = 1$ are easily comprehensible and in common use. The terms for $[j] > 1$, however, are somewhat ambiguous. In the present section, therefore, the terms *sublattice*, *coincidence lattice* or *twin lattice* of index [j] are preferred. Merohedral twinning is treated in detail in Section 3.3.9.

Complete and exact three-dimensional lattice coincidence ($[j] = 1$) always exists for inversion twins (of noncentrosymmetric crystals) [twin operation (vii)]. For reflection twins, complete or partial coincidence occurs if a (rational) lattice row [*uvw*] is (exactly) perpendicular to the (rational) twin reflection plane (*hkl*); similarly for rotation twins if a (rational) lattice plane (*hkl*) is (exactly) perpendicular to the (rational) twofold twin axis [*uvw*].

The systematic perpendicularity relations (*i.e.* relations valid independent of the axial ratios) for lattice planes (*hkl*) and lattice rows [*uvw*] in the various crystal systems are collected in Table 3.3.8.1. No perpendicularity occurs for triclinic lattices (except for metrical accidents). The perpendicularity cases for monoclinic and orthorhombic lattices are trivial. For tetragonal (tet), hexagonal (hex) and rhombohedral (rhomb) lattices, systematic perpendicularity of planes and rows occurs only for the $[001]_{\rm tet}$ and the $[001]_{\rm hex}$ (or $[111]_{\rm rhomb}$) zones, *i.e.* for planes parallel and rows perpendicular to these directions, in addition to the trivial cases $[001] \perp (001)$ or $[111] \perp (111)$. In cubic lattices, every lattice plane (*hkl*) is perpendicular to a lattice row [*uvw*] (with $h = u$, $k = v$, $l = w$). More general coincidence relations were derived by Grimmer (1989, 2003).

The index [j] of a coincidence or twin lattice can often be obtained by inspection; it can be calculated by using a formula for the auxiliary quantity j' as follows: