o.m4.o3 **Twinning by syngonic, metric and selective merohedry, and their effect on the diffraction pattern**
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The classification of twinning by merohedry has been recently revisited[1,2] to include some cases absent in Friedel's analysis[3]. Commonly, the symmetry of the Bravais lattice corresponds to the holohedry of the syngony (crystal system) to which the space-group of the structure belongs, but in some cases it may accidentally correspond to a higher holohedry. For example, an orthorhombic crystal belongs to the orthorhombic syngony, to which the proper holohedry is *mmm* and usually the Bravais lattice is *oP* or *oS*. Let us suppose that the relation $b = a$ is accidentally obeyed, within the experimental uncertainties, by an orthorhombic crystal: the Bravais lattice of the crystal is *tP* or *tI* and has holohedry 4/*mmm.* The twin elements by merohedry, which in absence of the higher lattice symmetry would belong to the *mmm* holohedry, have to be subdivided into two kinds, depending on whether they belong to both *mmm* and 4/*mmm* holohedries or only to 4/*mmm.* The latter case is termed *metric merohedry* (class IIB) and corresponds to the degeneration of reticular merohedry to twin index 1 or of pseudo-merohedry to zero obliquity. The former corresponds to the classic merohedry[3] and is called *syngonic merohedry* (class I for hemihedral non-centrosymmetric crystals; otherwise class IIA)[2,4]. A class IIB twin generally gives a diffraction pattern with a metric symmetry higher than the syngony obtained from the intensity distribution, and non-equivalent reflections are overlapped with consequent problems in the crystal structure determination.

When twinning by merohedry involves an OD structure (*i.e.* a polytype in which the layer pairs are geometrically equivalent)[5] the twin law may belong or not to the point group of the family structure, *i.e.* the fictitious structure obtained by completing all the space groupoid operations of the polytype to space group operations. Correspondingly, twinning is subdivided into *selective merohedry* and *complete merohedry*. Twinning by *selective merohedry* corresponds to reticular merohedry for the family structure but to merohedry for the OD structure. It produces violation of some of the non-space-group absences typical of the OD structure, by overlapping present reflections of one individual to absent reflections of another individual, modifying thus the geometry of the diffraction pattern. If the OD character of the structure is known the presence of twinning by selective merohedry clearly appears at simple inspection[1].

[1] Nespolo M., Ferraris G., Durovic S. "OD character and twinning – Selective merohedry in class II merohedric twins of OD polytypes". Z. Kristallogr., 1999, 214: 776-779.
[2] Nespolo M., Ferraris G. "Twinning by syngonic and metric merohedry. Analysis, classification and effects on the diffraction pattern". Z. Kristallogr., 2000, 215: 77-81.
[3] Friedel, G. (1926). *Leçons de Cristallographie*, Berger-Levrault: Nancy, XIX+602 pp.
[4] Catti M., Ferraris G. "Twinning by Merohedry and X-ray Crystal Structure Determination". Acta Crystallogr. 1976, A32: 163-165.
[5] Dornberger-Schiff, K. (1964). *Grundzüge einer Theorie von OD-Strukturen aus Schichten.* Abh. dtsch. Akad. Wiss. Berlin, Kl. f. Chem. 3. 107 p.

o.m4.o4 **Tensor Calculus of Twinning.**
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In the following we consider a pair of orientation states S_1 and S_2 which are connected by transformation g so that $S_2 = gS_1$. If the symmetry of the state S_1 is F_1, then symmetry of the state S_2 is $F_2 = gF_1g^{-1}$. The ``*twinning group*'' $K = \{F_1,g\}$ is defined as the group generated by the symmetry F_1 and by the twinning operation g. Notice that it is also $K = \{F_1,g^{-1}\} = \{F_2,g^{-1}\} = \{F_2,g\}$. The two states can be formally considered as a pair of domain states arising in a structural phase transition in which the twinning group K plays the rôle of the parent group, while the groups F_1 and F_2 represent the low symmetry groups.

Domains pairs can be now classified into four types depending on the double coset F_1gF_1 which can be either ``*simple*'' or ``*multiple*'', and ``*polar*'' or ``*ambivalent*''. Up to this point we can use this approach in structural studies where F_1 and F_2 are space groups and g is an isometry. The first step in an analysis of posssible structure of interfaces between S_1 and S_2 is to find the distinction between the two states. A method has been developed for macroscopic (continuous) approximation where F_1 and F_2 are point groups and is a point operation.

Distinction of the two states by their macroscopic (tensorial) properties is determined by a two-step method. Tensors of interest are decomposed into their covariant components which transform as the bases of ireps (real ireducible representations) of the twinning group. These components are linear combinations of cartesian components and they can be interpreted as tensor parameters of domain states. In the first step, called ``*labelling of covariants*'', certain symbols are assigned to these parameters. In the second step, ``*conversion equations*'' are found in which cartesian components are expressed as linear combinations of these parameters. These equations facilitate consideration of the change of material properties on a path across the domain wall or twin boundary. They represent, in a certain sense, the basic equations of tensor calculus for an analysis of ferroic transitions and twinning.

Information about explixit tensor characteristics of domain states for tensors up to fourth rank is prepared in the form of a software which covers all symmetry descents between crystallographic point groups. This will constitute part of a CD ROM supplement to Vol. D: ``*Physical Properties of Crystals*'' of the International Tables for Crystallography. This software will be demonstrated and possibilities of its extension to magnetic point groups and magnetic properties will be explained.