[MS36-02] Structural analysis of twinning: the example of melilite. Massimo Nespolo[1], Mohamed-Amine Marzouki[1,2,] Bernd Souvignier[2].

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The reticular theory of twinning, in its last extension known as theory of hybrid twins [1], provides the necessary conditions for the formation of a twinned crystal. These are based on the degree of restoration of the lattice under the action of the twin operation. The lattice nodes which are restored define a common sublattice across the interface between the individuals constituting the twin and a pre-requisite for the formation of the twin is given by the condition that the proportion of restored lattice nodes is high (at least 1/6 according to an empirical rule). But since the atomic structure does not possess the full symmetry of its lattice, the lattice restoration cannot discriminate twins of different compounds with the same type of lattice. This requires a structural approach [2] providing the sufficient conditions for the formation of a twin, which can be obtained by the following procedure. 1) Determine the intersection of the lattices of the individuals: this is the largest sublattice common to the twinned individualsand is called the twin lattice; 2) find the largest subgroup H of the space group G of the individual which is compatible with the twin lattice: this is obtained as the intersection of the space groups of the individuals (of the same type) in their respective orientations; 3) split the occupied Wyckoff positions of G into those of H and determine the crystallographic orbits under the action of H; 4) identify those crystallographic orbits under H which are restored by the twin operation, within a reasonable tolerance (pseudo-restored): this occurs when the eigensymmetry of the crystallographic orbit contains, exactly or as a pseudo-symmetry, the twin operation; 5) for a crystallographic orbit not restored by the twin operation, check whether it is mapped to a different orbit such that the union of these orbits is invariant under the twin operation: in this case, the eigensymmetry group of this union of orbits contains the twin operation, and it is this union of orbits which is restored. The proposed procedure is illustrated by applying it to the (100), (010) and (120) twins of melilite for which the eigensymmetry and restoration of crystallographic orbits is analysed .

[1] Nespolo, M, Ferraris, G (2006). Acta Cryst., A62, 336-349.
[2] Nespolo, M, Ferraris, G (2009). Eur. J Miner., 21, 673-690.

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