1.75: OD structure

OD structures consist of slabs with their own symmetry, containing coincidence operations constituting a diperiodic group(layer group) only within individual slabs. For the entire structure these coincidence operations are only local (partial), i.e. they are valid only in a subspace of the crystal space. The ambiguity (= existence of more than one equivalent possibilities) in the stacking of slabs arises from the existence of this local symmetry, which does not appear in the space group of the structure. The resulting structure can be "ordered" (*periodic*) or "disordered" (*non-periodic*), depending on the sequence of local symmetry operations relating pairs of slabs. The set of all the operations valid in the whole crystal space constitutes a space group; by adding the set of all the operations valid in a subspace of it, one obtains a space groupoid.

In the OD theory, a central role is played by the **vicinity condition** (**VC**), which states the geometrical equivalence of layer pairs. The vicinity condition consists of three parts:

- **VC α**: VC layers are either geometrically equivalent or, if not, they are relatively few in kind
- **VC β**: translation groups of all VC layers are either identical or they have a common subgroup
- **VC γ**: equivalent sides of equivalent layers are faced by equivalent sides of adjacent layers so that the resulting pairs are equivalent.

If the position of a layer is uniquely defined by the position of the adjacent layers and by the VC, the resulting structure is fully ordered. If, on the other hand, more than one position is possible that obeys the VC, the resulting structure is an **OD structure** and the layers are **OD layers**. VC structures may thus be either fully ordered structures or OD structures. All OD structures are polytypic; the reverse may or may not be true. Equivalency depends on the choice of OD layers and also on the definition of polytypism.