Keynote Lecture

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Crystallographic rationale for the formation of twinned crystals

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The reason why some crystals often occur as twins while others are rarely if ever twinned has intrigued investigators since the dawn of crystallography. The occurrence of growth twins often hampers the development of new materials with interesting physical properties and is a serious obstacle to the structural investigator. Understanding the structural reasons for the formation of twins opens the door to the development of protocols capable to reduce, if not eliminate, the occurrence of twins.
The reticular theory introduced by the French school established a relation between the occurrence frequency and the degree of lattice restoration [1] but cannot explain why some twins with the same degree of lattice restoration have a different occurrence frequency; it also cannot explain the occurrence of some (rarer) twins with low lattice restoration. The second problem was solved by the introduction of the theory of hybrid twins, where the existence of concurrent sublattices was recognized [2]. A more general approach was recently introduced, based on the analysis of the eigensymmetry of the crystallographic orbits [3]. A crystal structure can be decomposed in a number of crystallographic orbits, an orbit being composed by the atoms related by the symmetry operations of the space group G of the structure. Each crystallographic orbit possesses an eigensymmetry E which either coincides with G or is a supergroup of G. When E > G, we may find in E some operations (restoration operations), not contained in G, whose linear part coincides with the twin operation. If that is the case, then the corresponding orbit is not affected by the change of orientation produced by the twin operation and crosses the interface separating the twinned crystal without perturbation. When a significant subset of the crystallographic orbits possess one or more restoration operations in their eigensymmetry, then a substructure of the crystal structure crosses without perturbation the interface and represents the structural justification for the formation of the twin.
Quite often, the eigensymmetry E containing a restoration operation is only a pseudo-symmetry; at the interface, the corresponding substructure does undergo some deformation, which is however small enough to explain the formation of the twin.
A series of examples will be presented where the eigensymmetry of the crystallographic orbits stands out as the factor behind the formation of twins.

[1] Nespolo, M. (2015). Cryst. Res. Tech. 50, 362-371.
[2] Nespolo, M., Ferraris, G. (2006). Acta Cryst. A62, 336-349.
[3] Marzouki M. et al. (2014) IUCrJ 1, 39-48.
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