MS44-03 | The Need for Correlation Coefficients in the Modeling of Stacking Faulted Crystal Structures

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Standard refinement programs restrict the user to a model that allows twinning of a partially disordered average structure. However, there are structures where there are alternative relationships between adjacent ordered layers and this allows regions of commensurately related ordered structure with different origins, different orientations and different space groups. Each region can be described as a different occupancy modulation of an equally disordered structure of higher symmetry with subsequent atom displacements consistent with the local space group defined by the relative positions of immediately adjacent layers. Specific reflections can have contributions from different numbers of the component structures. The diffraction pattern identifies unit cells consistent with the options to be considered.

Locally the structure factor is $F(\mathbf{h}) = S_n P_n F_n(\mathbf{h})$ so that averaging over the crystal

$$|F(\mathbf{h})|^2 = S_n [<P_n^2> |F_n(\mathbf{h})|^2 + S_{m>n} <P_m P_n> [F_m(\mathbf{h})^* F_n(\mathbf{h}) + F_m(\mathbf{h}) F_n(\mathbf{h})^*]]$$

where $<P_m P_n> = X_{mn} [<P_n^2><P_n^2>]^{1/2}$

Twinning and allo twinning imply a correlation coefficient X_{mn} of 0, ie sample regions see only a single structure in a single orientation and intensities are a sum of component intensities. Correlation coefficients of 1.0 imply sample regions all see the same average disordered structure. Reality is often somewhere in between and this can be seen by using separate scales for data with different index conditions and for differences in pseudo equivalent reflections using a prototype structure that is a mixture of the space group options described using a space group that only includes the symmetry elements the options have in common. Worked examples will be given.