

Stacking faulted crystal structures can require correlation coefficients in their modeling.

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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 a 1:1 disordered structure of higher symmetry with subsequent atom displacements consistent with the local space group. The diffraction pattern identifies unit cells consistent with the options that need to be considered. Locally the structure factor is $F(\mathbf{h}) = \sum_n P_n F_n(\mathbf{h})$ so that averaging over the crystal

$$|F(\mathbf{h})|^2 = \sum_n [\langle P_n^2 \rangle |F_n(\mathbf{h})|^2 + \sum_{m>n} \langle P_m P_n \rangle [F_m(\mathbf{h})^* F_n(\mathbf{h}) + F_m(\mathbf{h}) F_n(\mathbf{h})^*]]$$

where $\langle P_m P_n \rangle = X_{mn} [\langle P_n^2 \rangle \langle P_n^2 \rangle]^{1/2}$

Allo twinning implies a correlation coefficient X_{mn} of 0, ie sample regions see only a single structure 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 enlightenment can be obtained 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.