OlexSys

The Twinning Problem

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OlexSys creates and maintains crystallographic software, enabling the structure solution and refinement of crystalline structures, through the use of X-ray diffraction.

When a crystal is in the path of a beam of X-rays, it diffracts them, causing bright peaks in particular directions. These directions can be seen as a lattice in reciprocal space, and have differing intensities.

In the case of twinning, there is an unknown 'rotated' component (or multiple) within the crystal, which leads to an identical rotation of the reciprocal lattice. This is then overlaid on the original lattice, and the intensities of points which land at the same spot are combined.

Frequently, these twins are not spotted at the point where one 'integrates' the frames to form this reciprocal lattice, and so any points which do not lie on that lattice are lost. Additionally, some points which do lie on the lattice may be artificially inflated in intensity, because more than one lattice may contribute to its intensity.

When we have a model for a structure, we can predict what the diffraction pattern for that structure would be.

We are interested in methods to identify twinned structures at this stage - when one has identified some (potentially systematic) ill-fitting reflections, and wishes to see whether there is any rotation R to the diffraction pattern which would cause other spots to overlay onto these underestimated (w.r.t the measured intensity) reflections. If one is found, we also need to evaluate how likely it is to actually be there - how much it mitigates for these underestimations, whether it overlays any other spots, and so on.

In its simplest format, given a lattice $\Gamma \subset \mathbb{R}^3$, we wish to find R such that certain lattice points of $R\Gamma$ are in sufficiently close proximity to ones of Γ. In the more complicated case, an R such that these points contain a particular pre-defined subset of Γ. We would also like to find quicker ways to evaluate the most effective such R.

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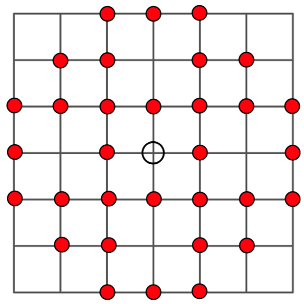

Figure 1: The diffraction of one component

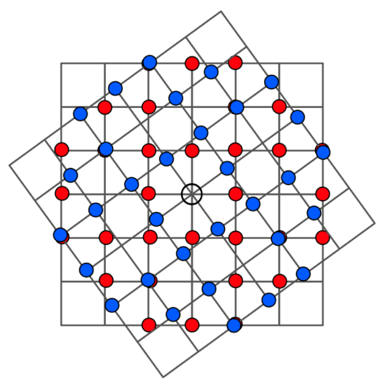

Figure 2: The diffraction patterns overlaid

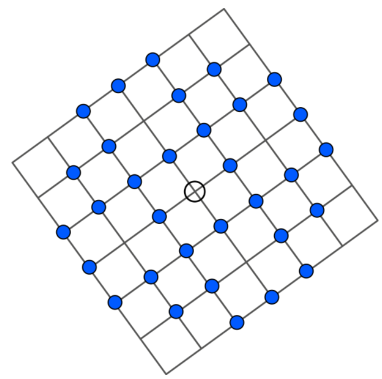

Figure 3: The diffraction of the twin

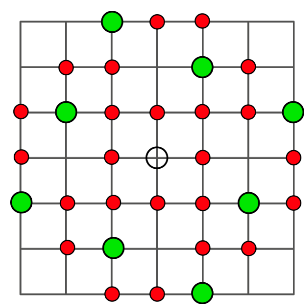

Figure 4: The final observed diffraction