MS45 What is inside the black box?

MS45-03

Efficient determination of possible twin laws using modified Rodrigues parameters

C.L. Hall [1], L.N. Midgley [2], C.G. Böhmer [3], N. Peyerimhoff [2], H. Puschmann [4]

[1]University of Bristol - Bristol (United Kingdom), [2]University of Durham - Durham (United Kingdom), [3]University College London - London (United Kingdom), [4]OlexSys - Durham (United Kingdom)

Abstract

In many situations, it is difficult to obtain crystals that produce perfect diffraction patterns and instead structures need to be determined using crystals with structures or defects that affect the diffraction pattern. One important example is twinning, which leads to the appearance of multiple sets of reflections associated with the different twin domains; represented in reciprocal space, these sets of reflections are related by rotation about the origin [1,2]. If the reciprocal lattices of the different twin domains do not overlap, then structure determination for a twinned crystal is relatively straightforward [1]. However, overlap of the lattices (especially the partial overlap associated with some non-merohedral twins) makes structure determination difficult as it is necessary to disentangle the data from the different twin domains [1,2]. We present a new method for determining twin laws that would lead to possible overlaps between the reciprocal lattices associated with different twin domains. This method depends on representing 3D rotations using "modified Rodrigues parameters" (MRPs), which are stereographic projections of the unit quaternions into 3D Euclidean space and which can be used to represent all 3D rotations [3]. Using MRPs, we have developed a computationally-efficient method that determines which rotations of a given reciprocal lattice could lead to some or all of the rotated reflections being within a specified tolerance of the original reflections. The error control on small perturbations in MRPs [3] means that we are guaranteed to find all possible twin laws that would cause a given number of rotated reflections to be within tolerance of the observed original reflections. The output of our algorithm is a list of possible twin laws in order of severity (i.e., the number of bad reflections that they would cause). These could then be used as twin candidates for further algorithms to perform the detwinning and automatically correct the integration of the bad reflections.

References

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