MS26 Quantum mechanical models for dynamics and diffuse scattering

MS26-02
Solution of single-crystal diffuse scattering problem using 3DΔPDF deconvolution
A. Simonov [1], Y. Kholina [2]

[1]Department of Materials, ETH Zurich - Zurich (Switzerland), [2]Department of Materials, ETH Zurich - Zürich (Switzerland)

Abstract
Properties of many materials depend crucially on the structure and distribution of defects in their crystal lattice. Defects can be probed by single crystal diffuse scattering of X-rays or neutrons, however the problem of construction of a model disordered solid consistent with the observed diffuse scattering is still unsolved since currently it relies on either trial-and-error or Patterson function based methods. Ideally one would seek a method which would allow to solve diffuse scattering in the same sense as direct methods provide a solution to the phase problem of the Bragg peaks crystallography.

In this work we show that such a general method indeed exists for the special case of binary disordered solids. Our method relies on the deconvolution of the 3DΔPDF function into two parts: one encoding the structure of the defect, and the other encoding the correlation between defects. The structure of the defect can then be solved by using standard algorithms similar to charge flipping, while the interaction between the defects can be found using the method called the density consistency matching. We illustrate the use of the method using the experimental data from tris-tert-butyl-1,3,5-benzene tricarboxamide single crystal.