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Single crystal diffuse scattering for analyzing structures of dilute defects

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With the recent advances in synchrotrons and area detectors, high quality single crystal diffuse scattering datasets can be routinely measured in a matter of minutes. However, analysis of diffuse scattering is still a bottleneck. It often requires construction of multiple test models and complicated refinements, and typically takes months of work and tens of thousands of computer hours.

Recently it was shown that in favourable cases of translational disorder diffuse scattering can be analyzed analogous to the Bragg peaks[1]. In such cases diffuse scattering can be used as a 'virtual structure factor', which can be combined with conventional structure factor to improve the resolution of refined atomic structure.

In the present contribution we extend this approach to the case of crystals with dilute defects. We show how information about defect distribution can be deconvolved from the virtual structure factor, and how the structure of defect can be found from diffuse scattering alone, without the use of Bragg peaks.

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