Deterministic Bragg Coherent Diffraction Imaging: Kinematical approximation

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A deterministic variant of Bragg Coherent Diffraction Imaging is introduced [1] in its kinematical approximation, for X-ray scattering from an imperfect crystal whose imperfections span no more than half of the volume of the crystal. This approach provides a unique analytical reconstruction of the object's structure factor and displacement fields from the 3D diffracted intensity distribution centred around any particular reciprocal lattice vector. The simple closed-form reconstruction algorithm, which requires only one multiplication and one Fourier transformation to be applied to the diffracted 3D intensity distribution, is not restricted by assumptions of smallness of the displacement field. The algorithm performs well in simulations incorporating a variety of conditions, including both realistic levels of noise and departures from ideality in the reference (i.e. imperfection-free) part of the crystal.

References

1. Pavlov K.M., Punegov V.I., Morgan K.S., Schmalz G., Paganin D.M., «Deterministic Bragg Coherent Diffraction Imaging», *Scientific Reports*, 7, 1132 (2017).