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# A method to correct angular distortions in Bragg Coherent X-ray Diffraction Imaging

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Bragg Coherent Diffraction Imaging (BCDI) is a powerful X-ray imaging technique to reveal 3D strain distribution of crystalline nanoparticles. The method records the 3D diffraction intensity of a nanoparticle slice by slice by incrementally rotating the sample within a very small angular range. The iterative phase retrieval method will then be employed to phase the sampled 3D diffraction intensity and provides the detailed three-dimensional (3D) distribution of strain. Thanks to the coherence produced by the latest $4^{th}$ generation of highly brilliant X-ray beams, BCDI can achieve a very high spatial resolution. However, any angular distortions from nominal rocking angles due to factors like the radiation heating, pressure or the imprecise rotation stage in the data acquisition process can introduce the artifacts in the following phase retrieval, which limits the applicability of BCDI. This prevents us from exploring more in material science, especially for the case of small nanoparticles.

In this study, we introduce a pre-processing algorithm designed to mitigate the impact of unexpected orientations. Inspired by the Extension-Maximize-Compress algorithm commonly employed in single particle x-ray imaging, our approach generates and refines a 3D diffraction intensity volume from measured 2D diffraction patterns. It achieves this by maximizing a likelihood function informed by Poisson statistics. This function includes cross-correlation between photon counts in each measurement and pixels in each slice of the generated volume, facilitating the determination of the relative orientation trajectory. Additionally, we further impose spatial constraint (envelope) on the 3D diffraction volume update, effectively limiting the field of view and enforcing the particle's maximum physical dimensions.

Our method demonstrates significant resilience to angular distortions, accurately correcting for distortions up to 16.4 times (1640%) of the angular step size $d = 0.004$ , which is comparable to the fringe spacing in our simulated dataset. The corrected result remarkably improves the quality of subsequent phase retrieval reconstruction, even in presence of Poisson noise.

The validation test underscores the potential of our pre-processing method to recover highly distorted experimental data that would otherwise be unusable. This advantage not only salvages data previously considered lost but also enhances the robustness of BCDI under less-than-ideal conditions. For example, our method can handle the data from the continuous scanning BCDI experiment.

In conclusion, the implications of this work extend to enabling BCDI in more demanding and challenging environments, fully leveraging the intensity of beam from $4^{th}$ generation synchrotrons, pushing the frontiers of material science research.

**Author:** CHEN, Huaiyu (Lund University)

**Co-authors:** DZHIGAEV, Dmitry; BJÖRLING, Alexander; WESTERMEIER, Fabian; LYUBOMIRSKIY, Mikhail; STUCKELBERGER, Michael; WALLENTIN, Jesper

**Presenter:** CHEN, Huaiyu (Lund University)

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