Bragg Coherent Diffraction X-ray Imaging of Nanoparticles with Unknown Orientation

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Bragg coherent diffraction imaging (BCDI) is a non-intrusive technique which enables mapping the internal strain fields of crystalline nanoparticles[1]. During BCDI experiments, the sample is oriented to a Bragg anglewith respect to an incoming X-ray beam, fulfilling Bragg's law. A detector measures the resulting Bragg peak and by controlled rotation of the sample along a rocking curve, the entire 3D diffraction volume can be reconstructed. The internal structure of the sample can be recovered by treatment of the diffraction volume via phase-retrieval algorithms.

Uncertainty in the sample's angular orientation during measurements, for example due to radiation pressure[2]or serial imaging schemes, can limit the applicability of BCDI. Methods proposed to overcome this limitation, such as ones based on the Expand-Maximize-Compress (EMC) algorithm, have shown success for angular deviations more than an order of magnitude of the nominal step size[3]. Even so, EMC is based on correlations between diffraction frames, complicating its extension to serial imaging methods where several single diffraction frames are measured from many identical but randomly oriented particles.

In this work, we propose a neural network (NN) which can predict the rocking angleof the sample based on individual diffraction frames, foregoing the need for continuity. Training the NN required no prior knowledge of internal strain and only an approximative shape of the measured particle. The network was tested on a merged dataset, containing diffraction frames (of unknown rocking angles) from three separate but similar~60 nm gold particles. The results showed that the NN was able to reconstruct a coarse sorting of the dataset, introducing continuity that the EMC algorithm could further refine to reconstruct the 3D diffraction volume. By enabling the treatment of datasets with unknown angular orientations and different particles, the proposed network helps bridge the gap toward serial imaging schemes in BCDI.

References

[1] G. J. Williams, M. A. Pfeifer, I. A. Vartanyants, and I. K. Robinson, "Three-Dimensional Imaging of Microstructure in Au Nanocrystals,"Physical Review Letters,vol. 90, no. 17, p. 175501, 04/29/ 2003.
[2] J. W. Kimet al., "Observation of x-ray radiation pressure effects on nanocrystals,"Journal of Applied Physics,vol. 120, no. 16, 2016.
[3] H. Chenet al., "Correcting angular distortions in Bragg coherent X-ray diffraction imaging,"Journal of Synchrotron Radiation,vol. 31, no. 5, pp. 1308–1316, 2024.