Mapping Data Between Sample and Detector Conjugated Spaces in Bragg Coherent Diffraction Imaging

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Bragg Coherent X-ray Diffraction Imaging (BCDI) is a non-destructive, lensless method for 3D-resolved, nano-scale strain imaging in micro-crystals. A challenge, particularly for new users of the technique, is accurate mapping of experimental data, collected in the detector reciprocal space coordinate frame, to more convenient orthogonal coordinates, e.g. attached to the sample. This is particularly the case since different coordinate conventions are used at every BCDI beamline, thus reconstruction algorithms and mapping scripts composed for individual beamlines are not readily interchangeable. We introduce a MATLAB BCDI experiment simulation with a plugin script that converts all beamline angles to a universal, right-handed coordinate frame, making it possible to condense any beamline geometry into three rotation matrices [1]. These matrices are implemented in MATLAB scripts that allow the user to map between various BCDI-related spaces, shown in Fig. 1, across different beamlines.

The ability to easily transform data between different spaces will be key for popularising BCDI, especially following the Extremely Brilliant Source (EBS) upgrade at the ESRF. The completion of the EBS upgrade at ESRF will see increased coherent flux, placing BCDI in a position to become a widespread imaging technique and microscopy tool for a general user community. In addition to simplifying space mapping, the scripts are also important for developing more robust phasing strategies, e.g. using projections from electron microscopy for phasing, and provides sample analysis flexibility, e.g. viewing the object in sample space or lab space. These tools are intended to serve as an initial toolkit for users to apply to various frameworks in their chosen disciplines. They can be downloaded from https://github.com/Hofmann-Group.

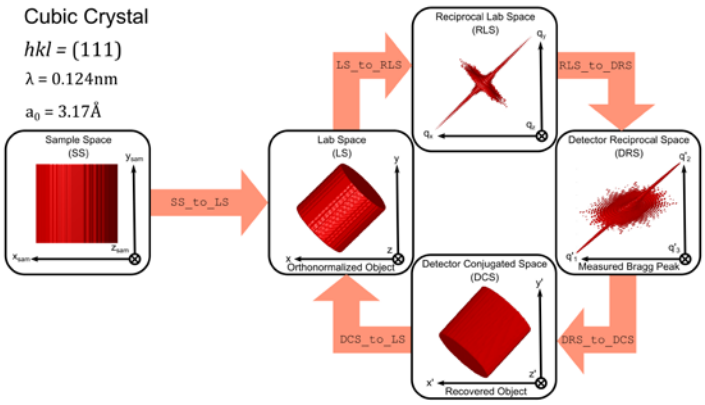

Figure 1: BCDI-related spaces in the MATLAB simulation [1] for a simulated cubic crystal cylinder at *hkl* = (111), a_0 = 3.17 ˚A and λ = 0.124 nm. MATLAB script filenames that convert from one space to another are shown inside the arrows.

References

[1] - D. Yang, N. W. Phillips, and F. Hofmann, *Mapping Data Between Sample and Detector Conjugated Spaces in Bragg Coherent Diffraction Imaging*. http://arxiv.org/abs/1906.12119, 2019.