Efficient ptychotomography methods for future high brightness X-ray sources

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Ptychographic X-ray computed tomography (PXCT) is a powerful method for nanoscale 3D imaging that can provide local quantitative values of the complex refractive index inside of a sample and an estimate of the local electron density. In particular, PXCT has a large potential for high resolution imaging in hard X-ray range, where the resolution was demonstrated down to 15 nm for highly scattering samples[1] and 28 nm for biological specimens [2].

On the other hand, high resolution PXCT imaging has severe limitations, in particular slow data acquisition compared to full field imaging, high computational costs and high radiation dose required for imaging that may result in radiation damage.

These limitations can become a major bottleneck with advent of the 4th generation X-ray sources that promise significantly lower emittance and in combination with other improvements in the beamline optics, increase of the available coherent X-ray flux by more than two orders of magnitude is expected. This results in an urge to develop a fast but still photon-efficient scanning method alongside with computationally efficient and noise-robust ptychographic reconstruction algorithms.

As a potential solution, we will present a recently developed method for arbitrary path fly-scan ptychography [3] that enables us to avoid limitations of the currently used fly-scan ptychography methods such as linear scan trajectory and at the same time to reach higher photon-efficiency, i.e. less photons are needed to reach the same reconstruction quality compared to the common fly-scan method. This improvement is combined with the newly developed approximation of the maximum-likelihood (ML) ptychography method [4] that lowers the per-iteration computational time and accelerates the convergence by an optimal selection of sub-sets of the scanning positions, applied sequentially or in parallel. In particular, faster convergence and lower per iteration computation cost for noise-limited datasets is important since the ptychographic reconstructions codes are nowadays often well optimized and significant speed up cannot be reached without changing the algorithms themselves.

The next major challenge is radiation damage of samples during PXCT scans. Radiation damage is a severe limitation particularly for high resolution imaging since the required imaging dose grows with more than 4th power of spatial resolution. For biological samples, radiation damage can be mitigated by cryo-protection [5], however even cryo-protected samples still often suffer from mild radiation damage [2]. In order to deal with that, we have developed a novel tomography reconstruction method that can account for small changes in the sample caused by radiation damage and attempt to estimate the original reconstruction of the sample before the dose was deposited. As we will demonstrate, the presented methods provide an improved reconstruction quality compared to the standard techniques, due to the use of a more optimal forward model for the PXCT task. This is especially important in the case of sample or illumination changes during the PXCT scan.

References