Poster Presentation

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Optimal data collection using photon-counting Hybrid Pixel Detectors

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The data collection parameters used in a diffraction experiment have a strong impact on the quality of the acquired data. A careful choice of parameters leads to better data and can make the difference between success and failure in phasing attempts and better data will also result in a more accurate atomic model. The selection of data acquisition parameters has to account for the application of the data in various phasing methods or high-resolution refinement. Furthermore, experimental factors like crystal characteristics and the properties of X-ray source and detector have to be considered. Hybrid Pixel Detectors are now for several years in use in macromolecular crystallography and an increasing number of synchrotron beamlines as well as laboratory instruments are equipped with such detectors. Photon-counting Hybrid Pixel Detectors have fundamentally different characteristics and offer various advantages over other detector technologies. To fully exploit the advantages of Hybrid Pixel Detectors, different data collection strategies than those established for other detector types have to be applied. Fine ϕ-slicing is a strategy particularly well suited because of the fast readout time and the absence of readout noise. This strategy was systematically investigated collecting a large number of data sets from crystals of four different proteins to investigate the benefit of fine ϕ-slicing on data quality with a noise-free detector in practice. The results show that fine ϕ-slicing can substantially improve scaling statistics and anomalous signal. Furthermore, when collecting data in continuous rotation at high frame rates up to hundreds of images per second, quality might be impaired by detector readout. Results on the influence of readout time on data quality will be presented and strategies to easily avoid detrimental effects of detector readout will be discussed.

Keywords: diffraction data collection, data-collection strategies, hybrid pixel detector