Contribution ID: **29** Type: **Invited**

Effects of dose control in multiple small wedge data collection

Wednesday, 14 October 2020 13:50 (20 minutes)

Recent brilliant micro-focused X-ray has enabled high resolution structural analyses of challenging biological proteins such from 10-μm sized crystals. One of the key technologies to achieve this is merging many partial datasets. This so-called 'multiple small wedge data collection'strategy was initially developed at Advanced Photons Source to accomplish data collection from in-meso phase crystals of membrane proteins. The loop containing several tens of tiny LCP crystals is raster scanned by low dose micro-focused beam. Based on this scan, crystals embedded in lipids invisible under the visible light are aligned to X-rays. From the angle where raster scan is applied, small wedge dataset is collected from each found crystal. Finally, many wedges from many crystals are merged into the final dataset.
At SPring-8, we have achieved to determine many membrane protein structures in this strategy. Recently, we developed ZOO system which enables un-attended fully automated data collection. The system has accelerated data collection in multiple small wedge scheme. A function to estimate absorbed dose for data collection is equipped to the system. Our recommended absorbed dose for all data collection scheme is 10 MGy under a cryo condition. It is based on our knowledge-based parameter in study of radiation damage by using micro-focused beam. However, no body have conducted the systematic study of effect of accumulated absorbed dose in 'multiple small wedge'strategy. In the full rotation data collection using a single crystal without any translation of irradiation points, radiation damage heterogeneously accumulated on the crystal volume and effects to errors in intensities in the identical dataset. On the other hand, multiple small wedge data collection is based on merging many datasets. In this case, merging equilibrates the radiation damage because heavily damaged data region is slightly compensated by another crystal with freshness against to the damage.
We systematically investigated effects of dose control in multiple small wedge data collection by using several standard protein samples. We will share our results to have discussions about the best dose for small wedge data collection.

Primary author: HIRATA, Kunio (RIKEN)

Co-authors: BABA, Seiki (JASRI/SPring-8); MIZUNO, Nobuhiro (JASRI/SPring-8); SAKAI, Naoki (RIKEN/SPring-8 Center); YAMAMOTO, Masaki (RIKEN/SPring-8 Center)

Presenter: HIRATA, Kunio (RIKEN)

Session Classification: Session 2 - Practical Aspects of Reducing Radiation Damage at Synchrotrons