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Investigation of radiation damage in room temperature serial macromolecular crystallography at a fourth generation Synchrotron

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Radiation damage is major concern in macromolecular crystallography (MX) where ionising X-rays used for structure determination can result in a cascade of damaging processes caused by the absorption of energy (denoted mainly as dose: absorbed energy/mass (J/kg; Gray (G)) and radiolysis of molecules. These can introduce artefacts within the structure (specific damage) and the overall data (global damage). Collection at cryogenic temperatures (100 K) is normally performed to mitigate the effects of radiation damage but recently there has been a resurgence in room temperature (RT) and serial crystallography collection. Serial synchrotron crystallography (SSX), with approaches adopted from X-ray free electrons lasers (XFELs), provides a suitable way to collect RT data at synchrotrons with reduced radiation damage by spreading the total dose over thousands of individual microcrystals. This usually relies on a microfocus beamline and a very low-dose per crystal collection strategy to compensate.

With advancements in technologies, synchrotrons are now being upgraded or constructed to fourth generation light sources, offering much higher brilliance compared to their predecessors, and, consequently, microfocus MX beamlines with increased flux density are becoming more routinely available offering much higher dose rates for RT-SSX collection. One example of this is ID29, the flagship beamline constructed at the high-energy fourth generation European Synchrotron Radiation Facility (ESRF), following its upgrade to the Extremely Brilliant Source (ESRF-EBS) [Raimondi et al, 2023]. ID29 is currently in unique territory, delivering slightly polychromatic (1% ΔE/E) microsecond X-ray pulses (90 μs) with a flux density of > 1014 ph/s/μm2, three times higher than third generation sources, and with dose rates on the order of several GGy/s. The unique beam characteristics on ID29 allow for the possibility of serial microsecond crystallography (SμX) for the structure determination of macromolecules using RT-SSX [Orlans et al, 2025]. As ID29 is setting a precedent for similar beamlines that are appearing or due to appear worldwide, a comprehensive radiation damage analysis is thus required.

References

[1] Raimondi et al. (2023) Communications Physics, 6, 82.
[2] Orlans et al. (2025) Communications Chemistry, 8, 6.

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Session Classification: Damage at New Sources - XFELs and 4th Generation Synchrotrons