



Contribution ID: 19

Type: **Invited**

Damage before destruction? X-ray-induced changes in single-pulse serial femtosecond crystallography

Tuesday 3 June 2025 17:15 (30 minutes)

Serial femtosecond crystallography (SFX) exploits extremely brief X-ray free-electron laser pulses to obtain diffraction data before destruction of the crystal. However, during the pulse X-ray-induced site-specific radiation damage can occur, leading to electronic state and/or structural changes. Here, we present a systematic exploration of the effect of single-pulse duration and energy (and consequently different dose rates) on site-specific radiation damage under typical SFX room-temperature experimental conditions. For the first time in SFX we directly measured the photon pulse duration, varying from less than 10 fs to more than 50 fs, and used three pulse energies to probe in-pulse damage in two radiation-sensitive proteins: the iron-heme peroxidase DtpAa and the disulfide-rich thaumatin. While difference-map features arising from radiation damage are observed, they do not lead to significant change in refined atomic coordinates or key bond lengths. Our work thus provides experimental verification that average atomic coordinates are not significantly perturbed by radiation damage in typical SFX experiments.

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