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Modeling X-ray-Induced Heating at 4th-Generation MX Beamlines

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The transition from 3rd to 4th generation synchrotrons—featuring diffraction-limited storage rings—has significantly expanded future possibilities for macromolecular crystallography (MX). These upgrades, characterized by reduced source divergence and increased electron bucket capacity, have boosted brilliance by up to two orders of magnitude. As a result, next-generation MX beamlines, such as ID29 (ESRF-EBS), BioCARS (APS-U), and MicroMAX (MAX IV), now deliver fluxes approaching 10ˆ15 ph/s. These extremely high flux (EHF) beamlines are increasingly optimized for time-resolved MX, aiming for microsecond-scale resolution.

Operating in previously unexplored dose regimes (>50 GGy/s) raises new challenges. In my presentation, I would like to share our study that focuses on beam-induced heating in microcrystals (<25 µm) exposed to EHF conditions. Thermal modeling indicates that such dose rates may cause significant temperature rises, potentially impacting data quality. Mitigation strategies include using top-hat beam profiles and increasing both beam and crystal sizes to distribute dose more evenly. The proposed model serves as a tool to support experimental design and optimize conditions for high-flux time-resolved MX. This of critical importance for future multidimensional X-ray protein crystallography, especially in enzymology, where temperature is a key experimental variable. As such they will require precise temperature measurements, as even a small change in temperature can affect the catalytic activity of an enzyme.

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