[MS12–02] Get the most out of your precious crystal with three dimensional dose modeling.

Oliver B. Zeldin[a], Markus Gerstel[a], Sandor Brockhauser[b], John Bremridge[a], Elspeth F. Garman[a].

[a]*Department of Biochemistry, University of Oxford, United Kingdom*
[b]*EMBL, Grenoble, France*
E-mail: robert.zeldin@dtc.ox.ac.uk

A common challenge for macromolecular crystallographers is to solve a difficult crystal structure from one well-diffracting crystal amongst many poorly diffracting ones. This presentation is about how to make the best possible use of this limited diffraction volume using a newly developed metric: Diffraction Weighted Dose.

Radiation damage during the diffraction experiment fundamentally limits how much data can be collected from a given crystal, and can degrade the image quality or even entirely prevent an atomic model from being obtained (1).

Extensive work has been carried out to understand the dose-dependent decay of diffraction quality (2–5), and guidelines exist for upper limits on the acceptable dose under carefully controlled even dose conditions. However, when applied to 'real world' scenarios, where the strategy has to be optimised for data collection rather than for systematic investigations of radiation damage progression, these results are not generally applicable (6). For a typical data collection, with non-uniform illumination from an approximately Gaussian X-ray beam and crystal rotation, the dose is not distributed evenly throughout the crystal volume. Thus the guidelines developed for a single dose state resulting from a uniform beam profile are difficult to apply.

We present (i) results from using the program RADDOSE-3D (7) to optimally distribute dose within a crystal volume, and (ii) a new metric: Diffraction Weighted Dose, which faithfully describes the relative total diffraction efficiency (the loss of intensity relative to the original diffraction intensity of the crystal: I_n/I_1) for a dataset collected from an un-evenly exposed crystal. Together, these developments represent a vital step towards eliminating radiation damage as a source of experimental failure for macromolecular crystallography.

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