Abstract

What dose DOES a micro-crystal really absorb?

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Eighteen years of published research on radiation damage to samples held around 100 K during X-ray crystallography has resulted in thorough characterisation of the phenomenon. However, there are still perplexing questions left to be answered in terms of understanding some of the observed effects, and before crystal clear guidance can be given to experimenters on how to minimise them.

Our recent work has led to the identification of damage metrics for assessing the damage to a lone PDB deposition [RABDAM, 1] and in producing tools for objective analysis of electron density loss in difference maps [RIDL, 2] derived from radiation damage diffraction data series collected from single crystals. New developments of our program, RADDOSE-3D [3,4], will also be covered. RADDOSE-3D computes spatially and temporally resolved dose fields in irradiated crystals, since the redistribution and escape of energy carried by photoelectrons and fluorescent photons are now included in the code. The former affects the dose absorbed by microcrystals and an analysis of how, in practice, this could translate to the extension of crystal lifetime in X-ray beams will be presented.

[1] RABDAM: quantifying specific radiation damage in individual protein crystal structures.
Kathryn L. Shelley, Thomas P. E. Dixon, Jonathan C. Brooks-Bartlett and Elspeth F. Garman. J. Appl. Cryst (2018) 51, 552-559.
[2] RIDL: a tool to investigate Radiation-Induced Density Loss.
Charles S. Bury, Elspeth F. Garman. J.Appl. Cryst. (2018) under minor revision
[3] RADDOSE-3D: time- and space-resolved modeling of dose in macromolecular crystallography
Oliver B. Zeldin, Markus Gerstel and Elspeth F. Garman. J.Appl. Cryst. (2013) 46, 1225-1230.
[4] Estimate your dose: RADDOSE-3D. Charles S. Bury, Jonathan C. Brooks-Bartlett, Steven P. Walsh & Elspeth F. Garman Protein Science (2018) 27, 217–228