Poster Presentations

[MS12-P05] Exploring Relationships Between Diffracted Intensity Decay and a New Dose Metric.

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Radiation damage is one of the major limiting factors for crystallographers trying to collect useful data during macromolecular X-ray crystallography (MX) experiments at third generation synchrotron sources [1]. The dose received by the crystal has long been thought to be a good indicator of the extent of the global radiation damage, however it is only recently that adequate tools have been established to allow us to accurately measure the dose distribution within a crystal during an MX experiment. Analysis of various dose metrics described in [2], has resulted in us developing a new way of quantifying dose for unevenly irradiated crystals: the Diffraction Weighted Dose (DWD). Experiments conducted by Zeldin *et al.* (unpublished) were performed to test the robustness of this dose metric at describing the damage observed under different dose contrast regimes for fifteen different cubic insulin crystals. The resolution dependent form of the intensity decay with the DWD is explored here. Our findings confirm that the decay of diffracted intensity is exponential as a function of the DWD where the decay rate is dependent on the diffraction angle. Comparison of these findings with the room temperature (RT) dose decay models (DDM) proposed by Blake and Phillips [3] (and extended by Hendrickson (1976) [4]) and also Leal *et al.* [5] are tested against the data to determine whether their RT DDMs can be extended to describe resolution dependent diffraction intensity loss at cryotemperatures (100K). Results of these comparisons show consistencies in the exponential form of the relationship between the diffracted intensities and the diffraction angle, and give some information on more appropriate DDMs that might be applicable across the entire range of intensity loss. These findings will be presented.

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