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Diffraction Intensity as a Radiation Damage Progression Metric and Intensity Decay Models

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Ever since the first systematic study of radiation damage in macromolecular crystallography, diffraction intensity decay has been useful as one of the metrics to monitor the progression of radiation damage in reciprocal space for room temperature [1] and cryo-cooled (˜100 K) [2] crystalline samples. Various models have been used to parameterise the functional form of the intensity decay (IDMs), but none thus far have been completely satisfactory in both fitting the data and having physically interpretable parameters. The absorbed dose is the most useful x-axis against which to plot intensity decay, since it allows different experimental arrangements to be compared, and the program RADDOSE-3D [3,4] was developed to allow convenient dose estimation.

Results from the recent inclusion of the option to enter an IDM [5] into RADDOSE-3D will be presented. The IDM enables the previous RADDOSE-3D output of 'Diffraction Weighted Dose'to be modified from a 'Fluence Weighted Dose'to a 'Diffraction-Decay Weighted Dose'[6], allowing more informed decisions to be made on possible data collection strategies. Over the last 10 years RADDOSE-3D [4] has been extended for use in a wide variety of diffraction and scattering experiments (MX, SMX, XFEL, SAXS, XPS, PXRD) and most recently, electron diffraction, RADDOSE-ED [6]. In addition, we have now released a new RADDOSE-3D GUI [6,7] which allows the estimation of dose for any of these modalities.

References

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