MS38-P03 | THE POTENTIAL BENEFITS OF USING HIGHER X-RAY ENERGIES FOR MACROMOLECULAR CRYSTALLOGRAPHY

Dickerson, Joshua (University of Oxford, Oxford, GBR); Garman, Elspeth (University of Oxford, Oxford, GBR)

Using X-ray energies higher than those normally used for macromolecular X-ray crystallography (MX) at synchrotron sources can theoretically increase the achievable signal as a function of dose and reduce the rate of radiation damage [1]. In practice, a major stumbling block to the use of higher X-ray energy has been the reduced quantum efficiency of silicon detectors as the X-ray energy increases, but hybrid photon counting CdTe detectors are optimised for higher X-ray energies, and their performance has been steadily improving. The potential advantages of using higher incident beam energy together with a CdTe detector for MX are explored, with a particular focus on the advantages that higher beam energies may have for MX experiments with microbeams or microcrystals. Our Monte Carlo calculations [2] show a greater than a factor of 2 improvement in diffraction efficiency when using microbeams and microcrystals of 5 μ m or less. These take into account the escape of photoelectrons from the crystal as well as entry from the surrounding material [3], both of which have now been incorporated into RADDOSE-3D.

- [1] Arndt, U. W. Optimum X-ray wavelength for protein crystallography. J. Appl. Cryst. 17, 118–119 (1984).
- [2] Dickerson, J.L. & Garman, E.F. (2019) J. Synchrotron Rad. in press
- [3] Nave, C. & Hill, M. A. Will reduced radiation damage occur with very small crystals? *J. Synchrotron Radiat.* **12**, 299–303 (2005).