Optimised high energy data collection in protein crystallography with a CdTe based detector

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The global need to collect diffraction data from micro-crystals has been reflected by the development of dedicated microfocus beamlines for macromolecular crystallography worldwide. The increased intensity and brightness of these beamlines imposes a fundamental limitation however which precludes successful structure determination from a single microcrystal: radiation induced damage. X-ray induced radiation damage means that data must often be merged from many crystals to yield a complete dataset for structure solution [1, 2]. This is frequently the case for challenging projects when only crystals of limited size are available. Increasing the X-ray energy beyond the typical 10-15 keV range promises to provide a solution to this problem via an increase in the amount of information that can be obtained per unit absorbed dose or 'diffraction efficiency' [3-5].

To date however hardware limitations have negated any possible high energy gains. Typically the sensor material of detectors used in macromolecular crystallography is silicon. With its low atomic number, silicon becomes transparent as the X-ray energy is increased and the detector quantum efficiency falls rapidly as a function of energy. Recently, detectors using cadmium telluride as a sensor material have been developed; resulting in a quantum efficiency of 90% below the cadmium absorption edge (26.7 keV) and nearly 80% up to energies of 80 keV [6].

Through use of a new cryogenic permanent magnet undulator and a Cadmium Telluride Eiger2 detector high photon fluxes at high energies (>20 keV) can be generated and resulting microcrystal diffraction efficiently detected. Our results show that at higher energies fewer crystals will be required to obtain complete data, as the diffracted intensity per unit dose increases significantly between 12.4 and 25 keV. In an additional gain for the crystallographer, we observe that data collected at higher energies typically extend to higher resolution. Taken together our results illustrate that the use of high energies allows the best possible data to be collected from small protein crystals pointing to a high energy future for synchrotron-based macromolecular crystallography.

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