Radiation decay of thaumatin crystals at three X-ray energies

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Radiation damage is an unavoidable obstacle in X-ray crystallographic data collection for macromolecular structure determination, so it is important to know how much radiation a sample can endure before being degraded beyond an acceptable limit. In the literature, the threshold at which the average intensity of all recorded reflections decreases to a certain fraction of the initial value is called the 'dose limit'. The first estimated D50 dose-limit value, at which the average diffracted intensity was reduced to 50%, was 20 MGy and was derived from observing sample decay in electron-diffraction experiments. A later X-ray study carried out at 100 K on ferritin protein crystals arrived at a D50 of 43 MGy, and recommended an intensity reduction of protein reflections to 70%, D70, corresponding to an absorbed dose of 30 MGy, as a more appropriate limit for macromolecular crystallography. In the macromolecular crystallography community, the rate of intensity decay with dose was then assumed to be similar for all protein crystals. A series of diffraction images of cryocooled (100 K) thaumatin crystals at identical small, 2° rotation intervals were recorded at X-ray energies of 6.33, 12.66 and 19.00 keV. Five crystals were used for each wavelength. The decay in the average diffraction intensity to 70% of the initial value, for data extending to 2.45 Å resolution, was determined to be about 7.5 MGy at 6.33 keV and about 11 MGy at the two higher energies.

References

[1] D. Liebschner, G. Rosenbaum, M. Dauter and Z. Dauter (2015) Radiation decay of thaumatin crystals at three X-ray energies, Acta Cryst. D71, 772-778.

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