Synchrotron radiation in crystallography: instrumentation, methods and applications

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ABSTRACT

I will give an overview of the developments in macromolecular crystallography (MX) synchrotron radiation crystallography, from my work at the first dedicated source at the SRS in Daresbury, UK, including the planning and early developments and applications at the 3rd generation SR X-ray source ESRF. The build of dedicated beamlines for resonant anomalous scattering phasing, the ability to handle large unit cells, high resolution and use of small crystals were key benefits. Chemical crystallography uses of SR were very important spin off developments of the SRS MX and applied notably to make feasible X-ray diffraction from very small crystals and the use of multiple wavelength anomalous dispersion. To advance towards structure solution from ever smaller samples MAD phasing for ab initio structure determination from powder diffraction data was instigated; the methods learnt are extendable to single nanoclusters at eg the next generation X-ray, SR and / or laser, sources. The development of the Laue method with SR was an unexpected development and has allowed pioneering steps in micro-crystallography, applications to time-resolved structural studies and also for reactor and spallation source neutron macromolecular and chemical crystallography. Crystal perfection and radiation damage studies of crystals have been an underpinning interest throughout. In Manchester these new methods have been further developed and applied in structural studies of sugar molecular recognition in concanavalin A, hydroxymethylbilane synthase enzyme catalysis and the coloration of the multi-protein complex crustacyanin with up to sixteen astaxanthins. The crustacyanin structural studies have expanded to include small-angle scattering, electron microscopy, chemical crystallography and spectroscopy of the astaxanthin enolate anion. There is an effective global cooperation of SR and neutron beamline and crystallography scientists, which has ensured a speedy and effective growth of crystallography at the facilities. I heartily thank my colleagues, my PhD students and PostDocs, and the SR and neutron facilities for their collaboration these last four decades.