[MS31-P04] Dynamic Structural Science: Diffraction Methods

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Diffraction methods have been extremely successful in the determination of time-averaged structures. Several techniques have been used in the past for the direct observation of reactions by crystallography, but only applied to very specific systems.

One of the objectives of the Dynamic Structural Science (DySS) consortium is to develop instrumentation and software that can be incorporated into any modern beamline allowing the collection of time resolved structural data. Based at the Research Complex at Harwell, the consortium brings together researchers from a wide range of structural backgrounds as well as beamline scientists from Diamond Light Source and ISIS, creating the opportunity to design and fine-tune experiments that will lead to our goal.

A chopper system has been installed on I19, the small molecule beamline at Diamond Light Source. Existing pump-probe methods for reversible systems have already been successfully applied to observe excited states with lifetimes in the ms range, and the current setup will allow us to move to the μs regime. Using a two-chopper system we will be able to select single bunches and thus reach ps timescales.

For non-reversible systems we are developing novel pump-probe methods using statistical analysis of data from many micro-crystals. At the I24 microfocus beamline, a single XRD shot is taken at desired time delays after photoactivation of a single crystal. A large number of crystals will need to be exposed to give sufficient coverage of reciprocal space and to allow for meaningful statistical analysis. Though applications using this methodology on I24 have to date focused on macromolecular systems, we will extend these to the small molecular chemical materials.