MS3-P12 Rapid data acquisition using an ultrasonic acoustic levitator and a next-generation pixel detector at room temperature

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A new data acquisition method was developed using an ultrasonic acoustic levitator and a next-generation pixel array detector in order to collect dataset rapidly at room temperature. Spinning of crystals in the levitated liquid droplet caused by the acoustic streaming and a rapid frame rate of few thousand Hz with the Eiger X detectors allow us to collect a dataset less than few hundred millisecond. We conducted the proof of principle experiments using lysozyme crystals and demonstrated the successful solution of the crystal structure. No damage due to the acoustic pressure was observed. Diffraction experiments were set up at the beamline X06SA, Swiss Light Source, Paul Scherrer Institut. Diffraction images were collected at 133 Hz with the Eiger X 16M detector and processed by CrystFEL data processing suite because of a smooth transition of rotation axis during the exposure. Details of the diffraction experiments, comparisons of structures solved by different methods and possible applications with this method will be presented.

Keywords: acoustic droplet levitation, room temperature, pixel array detector

MS3-P13 Big EP: Automated structure solution pipeline deployment at Diamond Light Source

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Automated processing of macromolecular crystallography data is an important component in effective use of valuable synchrotron beamtime. Providing feedback to experimenters during data collection allows better decision making regarding quality of their samples and experimental setup. The combination of increasing computational power and the development of automated structure solution pipelines makes it feasible to attempt solving structures during experimental sessions. Extensive computational and storage facilities at Diamond Light Source[1] has enabled deployment of a sophisticated data processing infrastructure[2-4]. Big EP is the latest in this line of software packages at Diamond that attempts to extend and exploit these resources to automatically build macromolecular models using the autoSHARP[5], Phenix AutoSol/AutoBuild[6,7] and Crank2[8] structure solution pipelines. Output of multiple trials using the SHELX[9] software suite and experimental records available in ISpyB[2] database are extensively used to identify datasets that pass selection criteria and to infer required input parameters for running the pipelines. Current computing infrastructure at Diamond results in Big EP successfully handling around one hundred suitable datasets a week and has provided users with useful starting models for further refinement.

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Keywords: macromolecular crystallography, automated structure solution, parallel computing