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The design of a TOF neutron diffractometer providing high availability with the combined use of X-ray and neutron scattering from a protein single-crystal with large unit cells

There are so many proteins which are embedded into biological membranes. Many membrane proteins are the major players in important cell processes and therefore key targets for research on human health and drug development. The crystals of these large membrane proteins typically have very large unit cells with repeat of a few hundred Å. Neutron diffraction experiments on membrane proteins can be used to unravel the catalytic mechanism of reactions involving water and the structure of the solvent. It is proposed to develop a dedicated best-in-class high throughput and high resolution time-of-flight single-crystal biomacromolecular neutron diffractometer at the JSNS. A new diffractometer is being designed to be able to collect a full hemisphere of Bragg data with a resolution 1.5 to 2 Å on a crystal over a lattice constant 250 Å. A new diffractometer bristles with a spherical array of over 40 detectors, all pointing inward to enclose a basketball-sized chamber where the pulsed neutron beam collides with the crystal sample. The neutron detectors are inserted through openings in two aluminium hemispheres, which can be pulled apart for access to the interior, the hemispheres themselves are on sturdy support structures. The sample mounted on the goniometer would be maintained inside the aluminium spherical sample holder filled with helium gas or under the vacuum to improve the signal to noise ratio. The average intensity of a Bragg peak decreases as the number of peaks increase with large unit cells. After neutron diffraction measurement, the sample could be transported into X-ray diffractometer in 2nd floor through the top loading cryostat while being kept frozen during the transportation. The sample could be exposed to the X-ray beam and the full data collections could be carried out at once. We show that this new experimental system is designed to provide higher throughput and efficiency for the simultaneous structure refinement of large biomacromolecules with two different quantum beams.

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