Design of a new single-crystal neutron time-of-flight diffractometer in J-PARC/MLF to realize large biomacromolecular structure analyses

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Neutron protein crystallography is expected to contribute to the elucidation and improvement of protein function through providing structural information of hydrogen atoms and water hydration. However, recent neutron diffractometers installed at the reactor and pulsed neutron facilities does not cover proteins with a large unit cell volume, especially membrane proteins and protein complexes.

From requests of structural biology community, we aim to build a high-resolution neutron time-of-flight diffractometer for biomacromolecule, which allows us to collect neutron diffraction data from crystals with unit cells even over 250 Å, at MLF in J-PARC. We chose a decoupled liquid hydrogen moderator as an appropriate source for this high resolution diffractometer from both view points of flux and pulse width to realize the data collection covering a full hemisphere of Bragg data to 2.0 Å resolution with a lattice constant over 250 Å [1]. At a given resolution ($\Delta d/d$=1 %), the diffractometer is designed to archive the highest throughput, minimal peak overlap and high signal-to-noise ratio by using a large wavelength bandwidth of neutrons sorted by time-of-flight (TOF) and an array of high spatial resolution (2.5 mm spatial resolution) position-sensitive area scintillation detectors covering a large solid angle.

The angular resolution affecting the instrumental resolution ($\Delta d/d$) will dominates at low angles, but becomes vanishingly small at high (back-scattering) angles. Consequently, flight path dependency of the time resolution against the scattering angle becomes more pronounced with increasing scattering angle. Therefore, it is beneficial to take as long flight-path length L_1 as possible in designing a new diffractometer for samples with large unit cells, while this comes at the expense of reduced bandwidth and at the expense of much higher cost for the instrument (longer neutron guide, much larger shielding volume). Here, we introduce the general plan for the beam line components and the experimental cave, including the result of Monte Carlo simulation using the McStas software package.

References [1] K. Tomoyori, *et al*, *J. Struct. Funct. Genomics*. (2014).