

Poster Presentation

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Neutron diffractometer covering protein crystals with large unit cell at J-PARC

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The structural information of hydrogen atoms and hydration waters obtained by neutron protein crystallography is expected to contribute to elucidation of protein function and its improvement. However, many proteins, especially membrane proteins and protein complexes, have larger molecular weight and then unit cells of their crystals have larger volume, which is out of range of measurable unit cell volume for conventional diffractometers. Therefore, our group had designed the diffractometer which can cover such crystals with large unit cell volume (target lattice length: 250 Å). This diffractometer is dedicated for protein single crystals and has been proposed to be installed at J-PARC (Japan Proton Accelerator Research Complex). Larger unit cell volume causes a problem to separate spots closer to each other in spatial as well as time dimension in diffraction images. Therefore, our proposed diffractometer adopts longer camera distance (L2 = 800mm) and selects decoupled hydrogen moderator as neutron source which has shorter pulse width. Under the conditions that L1 is 33.5m, beam divergence 0.4° and crystal edge size 2mm, this diffractometer is estimated to be able to resolve spots diffracted from crystals with a lattice length of 220 Å in each axis at d-space of 2.0 Å. In order to cover large neutron detecting area due to long camera distance, novel large-area detector (larger than 300mm × 300mm) with a spatial resolution of better than 2.5mm is under development. More than 40 these detectors plan to be installed, providing the total solid angle coverage of larger than 33%. For neutron guide, ellipsoidal supermirror is considered to be adopted to increase neutron flux at the sample position. The final gain factor of this diffractometer is estimated to be about 20 or larger as compared with BIX-3/4 diffractometers operated in the research reactor JRR-3 at JAEA (Japan Atomic Energy Agency) [1,2].

[1] I. Tanaka, K. Kurihara, T. Chatake, et al, *J. Appl. Cryst.*, 2002, 35, 34-40, [2] K. Kurihara, I. Tanaka, M. R. Muslih et al., *J. Synchrotron Radiat.*, 2004, 11, 68-71

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