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Toward construction of neutron diffractometer for protein crystal

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We performed a time-of-flight (TOF) single crystal neutron diffraction experiment with a diffractometer (the IBARAKI Biological Crystal Diffractometer (iBIX)) installed at a coupled moderator (CM) pulsed neutron source in J-PARC using single crystal silicon, and we determined several candidates for fundamental fitting functions to faithfully reproduce the TOF Bragg reflection profile asymmetries with the longer tail shape. The Vavilov and Landau distributions used to describe the energy loss of charged particles traversing a thin absorber were found to be in excellent agreement with the observed TOF profile. We are planning to design a new TOF single crystal diffractometer installed at a decoupled moderator (DM) pulsed neutron source in J-PARC. The peak profile provides narrow neutron pulses with short tail. In any event, however, it is expected that the Vavilov and Landau functions are very effective and appropriate for use in the TOF distribution of Bragg reflections because there is no fundamental difference in the neutron moderation process between the two kinds of moderator. It is possible to make use of these functions for the integration of Bragg reflection in the case of profile-fitting refinement for protein sample; these functions might also be applicable to peak separation of the overlapped Bragg reflection in the TOF direction in the foreseeable future.

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