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Design of a Single Crystal Macromolecular Neutron Diffractometer at the SNS. A.J. Schultz, P. Thiyagarajan, C. Rehm, J.P. Hodges, W.T. Lee, A.D. Mesecar, D.A. Myles, P.A. Langan, IPNS, Argonne Nat'l Lab, Argonne, IL 60439, USA.

Neutron Macromolecular Crystallography (NMC) is able to accurately determine proton locations, protonation states and hydration, and hydrogen/deuterium exchange in macromolecular crystals even at a moderate resolution (2 Å to 2.5 Å). In order to exploit the high neutron flux that will become available beginning in 2006 at the Spallation Neutron Source (SNS), it is proposed to develop a dedicated best-in-class high throughput and high resolution time-of-flight single crystal macromolecular neutron diffractometer (MaNDi) at the SNS. MaNDi is being designed to be able to collect a full hemisphere of Bragg data with a resolution of 1.5 to 2 Å on a crystal with a lattice constant up to 150 Å in a few days. A thorough evaluation of the instrument performance at different moderators using analytical equations and Monte-Carlo simulations show that the decoupled hydrogen moderator at SNS would be the best choice for MaNDi. State-of-the-art neutron guides and optics will be used for efficient beam transport and optimization of collimation at the sample. To reduce the radiation damage and the instrument background, a curved guide will be used to steer the beam gently so that the crystal will be out of line of sight of the moderator. The high throughput is accomplished by the use of a wide bandwidth of cold neutrons ($1.8 \text{ \AA} < \lambda < 4.5 \text{ \AA}$) sorted by time-of-flight and by an array of high resolution position-sensitive area detectors covering a large solid angle. It is expected that the unprecedented high data rates and resolution with MaNDi for the high resolution NMC will open up new avenues and greatly advance the field of structural biology.

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