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A High Resolution Macromolecular Neutron Diffractometer (MaNDi) at the SNS. A.J. Schultz¹, P. Thiyagarajan¹, C. Rehm², J.P. Hodges², D.A. Myles³, P. Langan⁴, A.D. Mesecar⁵, ¹IPNS, ANL, Argonne, IL 60439, ²SNS and ³CSMB, ORNL, Oak Ridge, TN 37831, ⁴Biosciences Div., LANL, Los Alamos, NM 87545, ⁵Center for Pharmaceutical Biotechnology, UIC, Chicago, IL 60607.

Neutron macromolecular crystallography can determine proton locations, protonation states and hydration, and hydrogen/deuterium exchange at even moderate resolution (2.0-2.5 Å). A time-of-flight single crystal macromolecular neutron diffractometer (MaNDi) is proposed to exploit the high neutron flux that will be available beginning in 2006 at the Spallation Neutron Source (SNS). MaNDi is being designed to collect data to a resolution of 1.5 to 2 Å on crystals with a lattice constants up to 150 Å. Optimization for high data rates and resolution will be 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. Simulations show that complete data sets can be measured for 0.1 mm³ size deuterated protein crystals in as little as a day. It is expected that the unprecedented higher data rates and resolution will greatly advance the fields of enzymology and drug development.

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