A Proposed Suite of Macromolecular Crystallography Facilities for NSLS-II

Lonny Berman,[1] Marc Allaire,[1] Mark Chance,[3] Wayne Hendrickson,[4] Annie Héroux,[2] Babu Manjasetty,[3] Allen Orville,[2] Howard Robinson,[2] Anand Saxena,[2] Dieter Schneider,[2] Wuxian Shi,[3] Alexei Soares,[2] Vivian Stojanoff,[1] and Robert Sweet[2]

(1) Brookhaven National Laboratory, National Synchrotron Light Source, Bldg. 725D, Upton, New York 11973, USA

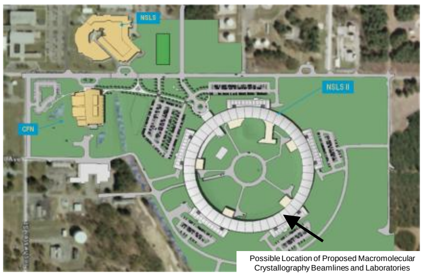
(2) Brookhaven National Laboratory, Biology Dept., Bldg. 463, Upton, New York 11973, USA

(3) Case Western Reserve University, Center for Synchrotron Biosciences, Cleveland, Ohio 44106, USA

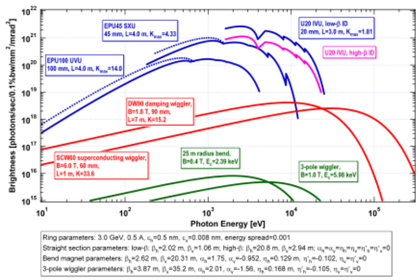
(4) Columbia University, Dept. of Biochemistry and Molecular Biophysics, New York, New York 10032, USA

A new, highly-optimized 3rd-generation synchrotron radiation (SR) source, the National Synchrotron Light Source -II (NSLS-II), is being planned as a replacement of the existing 2nd-generation SR source NSLS at Brookhaven National Laboratory (BNL). When NSLS-II becomes operational in 2015, it will deliver unprecedented brightness in the soft and hard x-ray spectral regions, about 10 times higher (at 8 keV) than the brightest SR sources now available.

Site Plan at BNL



Spectral Brightness of NSLS-II Sources



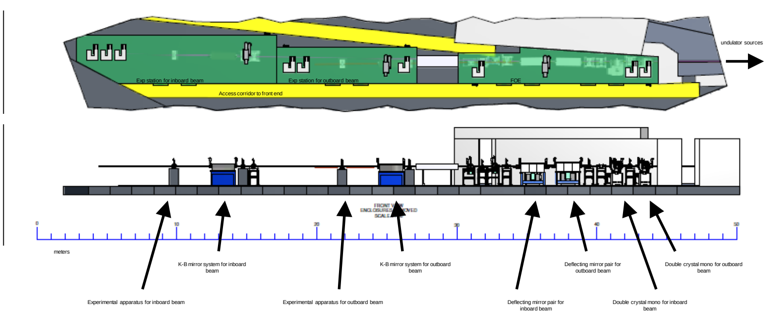
Storage Ring Parameters

3 GeV, 500 mA , top-off injection
Brightness > 10^{21} ph/sec/0.1%bw/mm^2/mrad^2
Flux > 10^{16} ph/sec/0.1% bw
Ultra-low emittance (ε_x, ε_y) 0.5 nm-rad horizontal, 0.008 nm-rad vertical
30 straight sections (15 low-β, 6.6 m long and 15 high-β, 9.3 m long)
30 bending magnets (25 m bend radius)
~15 three-pole wigglers

NSLS hosts a very strong macromolecular crystallography (MX) program, close to 40% of its user community. At NSLS-II, MX will be implemented in close association with other life sciences programs including small angle x-ray scattering, x-ray absorption spectroscopy, x-ray footprinting, and imaging at the nanoscale. It might be possible to co-locate the facilities which will support these life sciences programs in a "village" section of the NSLS-II facility to ensure that they are in close proximity.

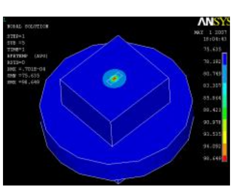
Possible Layout of a "Sector" of MX Beamlines

Here below we show how a pair of independent and tunable canted undulator MX beamlines might be laid out in the NSLS-II experimental hall. We are grateful to Lewis Doom and Michael Loftus of NSLS-II for furnishing this schematic, which emulates the GM/CA-CAT sector layout at the Advanced Photon Source (APS). We will investigate carefully this and other proposed designs for the MX beamlines, some of which might be optimized for special purposes.



Beamline Optics Challenges

The unprecedented brightness of NSLS-II undulators will impose strenuous demands on the quality of the optics in the beamlines. Simulations of the performances of silicon crystal monochromators and Kirkpatrick-Baez focusing mirror systems in an undulator beamline, shown below, highlight this. Research and development in implementing and assuring the quality of the optics will be necessary, and is planned.



Finite element analysis of a liquid nitrogen cooled silicon crystal exposed to the undulator beam indicates a slope error variation of ~10 μrad across the illuminated region of the crystal. Mitigating measures such as corrective optics and careful temperature monitoring and control will be explored and tested on existing NSLS beamlines.

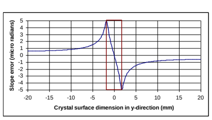


Table 11.3.1 NSLS-II Undulator-Based X-Ray Beamline Performance vs. Mirror Figure Error. The red (upper text line in each pair) signifies the "high" demagnification mode for this beamline, and the blue (lower text line) signifies the "low" demagnification mode.

RMS figure error [μrad]	0	0.1	0.5	1.0	2.0
Vertical focus size FWHM [μm]	1.0	2.6	11.8	23.5	47.0
	2.4	6.1	28.3	56.5	112.8
Horizontal focus size FWHM [μm]	15.5	15.8	21.0	32.2	58.5
	33.6	34.2	45.4	69.7	126.7
Monochromatic intensity at 12 keV [ph/s/μm^2]	1.0×10^{13}	4.5×10^{12}	7.9×10^{11}	2.7×10^{11}	7.7×10^{10}
	2.0×10^{12}	8.6×10^{11}	1.5×10^{11}	5.2×10^{10}	1.5×10^{10}

Note: FWHM = Full Width at Half Maximum

~ 2 orders of magnitude reduction in image flux density due to 2 μrad slope error compared with the 'perfect mirror', highlighting the importance of sophisticated mirror fabrication and metrology capabilities

Phased Implementation

The NSLS-II MX beamlines are proposed to be implemented in distinct phases spread over time:

Phase 1: Two brand new beamlines viewing U20 undulator sources installed in two sequential low-β straight sections and three beamlines derived from existing NSLS beamlines viewing three-pole wiggler sources

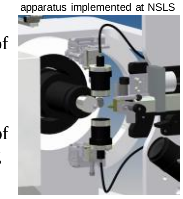
Phase 2: Two additional brand new beamlines viewing canted U20 undulator sources installed in the Phase 1 low-β straight sections

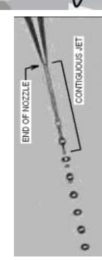
Phase 3: Two more brand new beamlines viewing canted U20 undulator sources installed in another low-β straight section

Endstation Challenges

Just as important will be the development of endstation equipment that will be able to cope with and exploit the brightness of NSLS-II undulators, including diffractometers which can handle crystals of microns dimension or smaller, fast-framing active-pixel detectors, automated sample exchange and cryogenic apparatus, and fluidic-based sample handling systems. New modes of data collection such as serial crystallography will have to be explored in order to overcome the effects of radiation damage. A range of spectroscopy capabilities concurrent with diffraction will be offered, including optical absorption, Raman, and fluorescence, all of which could be used on- or off-line. These will already become available at the existing NSLS facility.

combined diffraction - VUV/vis spectroscopy apparatus implemented at NSLS





"ink-jet" delivery of micro-crystals through the x-ray beam

D. Starodub et al., J. Synch. Rad. 15, 62-73 (2008)

For more information about NSLS-II, visit http://www.nsls2.bnl.gov. For more information about NSLS, visit http://www.nsls.bnl.gov. For more information about macromolecular crystallography at NSLS, visit http://www.px.nsls.bnl.gov. This work is supported by the U.S. Department of Energy and the U.S. National Institutes of Health.