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14. ABSTRACT

The funding from this Agreement was used to complete construction by the New York Structural Biology Center (NYSBC) of 'NYX' a new microdiffraction beamline at the National Synchrotron Light Source – II (NSLS-II) at Brookhaven National Laboratory (BNL). NSLS-II became the most advanced synchrotron in the world upon its completion in 2014, and NYX is a state-of-the-art beamline designed to exploit its unique capabilities. NYX will enable researchers to conduct crystallographic and biophysical experiments on a wider range of molecules than currently possible, including critical components in the activities of deadly viruses, biological toxins, and diseases

15. SUBJECT TERMS

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Proposal Number: 65277-CH, Agreement Number:W911NF-14-1-0110

Title: Completion of NYSBC Microdiffraction Beamline NYX

Authors: Hendrickson, Wayne A., and Lidestri, Joseph P.

Abstract

The funding from this Agreement was used to complete construction by the New York Structural Biology Center (NYSBC) of 'NYX' a new microdiffraction beamline at the National Synchrotron Light Source – II (NSLS-II) at Brookhaven National Laboratory (BNL). NSLS-II became the most advanced synchrotron in the world upon its completion in 2014, and NYX is a state-of-the-art beamline designed to exploit its unique capabilities. NYX will enable researchers to conduct crystallographic and biophysical experiments on a wider range of molecules than currently possible, including critical components in the activities of deadly viruses, biological toxins, and diseases including those used as biological warfare agents. The capabilities provided by NYX and the research that will be conducted at NYX, are of fundamental importance to national security.

Subject Terms

Synchrotron: particle accelerator that accelerates and stores electron beam at high energy for the purpose of generating x-ray radiation

Straight *section*: segment of the storage ring that accommodates insertion devices, notably undulators, that can produce brilliant x-ray beams

Beamline: instrumentation to focus, monochromatize, and safely control an x-ray beam

Canted beamlines: two beamlines emerging from a single straight section by virtue of canting magnets that divert the electron path into two slightly divergent directions

Undulator: periodic array of dipole magnets that oscillates the electron path whereby x-rays constructively interfere to enhance brilliance

Front End: instrumentation, including shutters, masks, slits and monitors, for the safe transport of x-rays between the undulator and the shield-wall port to the beamline

End Station: diffraction experiment instrumentation, including microdiffractometer system, robotic sample changing system, pixel array detector system, and data acquisition computing system

(Report for the period beginning March 15, 2014 and ending September 14, 2016)

The NYX beamline is designed to optimize three characteristics that address contemporary problems in biological crystallography: versatile focusing into microbeams of x-rays (5 – 50 μm cross-section) to analyze micron-sized crystals, tunability over a broad energy range (5 – 18 keV) for access to the electronic resonances of elements used in structure determinations by methods of anomalous diffraction, and high energy resolution (5×10^{-5} $\Delta E/E$) to optimize at-resonance anomalous scattering strength for use in phase evaluation. To achieve these features, high-precision optical components are required throughout and control systems are needed to assure high stability. The beampath is kept at ultra-high vacuum and must meet stringent standards for radiation safety. The NYX beamline comprises components inside the accelerator shield wall, including the undulator and front end, as well as certain components outside the shield wall, including radiation enclosures, beam transport assembly, beam delivery system, and experiment end station. NYX is a canted beamline that will share the insertion device (ID) straight section of NSLS-II 19-ID with beamline LAX for Low-energy Anomalous X-ray Diffraction, and the infrastructure for NYX must accommodate the canting mechanisms and dual front end components that are needed to deliver the beam to NYX while preserving the opportunity for future LAX development.

NYX is an NSLS-II Partner User Beamline. It is associated intimately with the NSLS-II synchrotron storage ring, and its construction required close coordination between NYSBC and NSLS-II. We established a Beamline Development Group (BDG) for the construction of NYX, and this group of NYSBC and NSLS-II personnel met regularly throughout this period of ARO support to develop and implement construction plans. We also developed a Project Management Plan (PMP), a Partner User Agreement (PUA), and a Strategic Partnership Project (SPP) Agreement. Although the majority of NYX beamline components were contracted directly by NYSBC or designed and implemented by NYSBC staff, work on those components directly related to accelerator performance, notably all components inside the accelerator shield wall and certain components related to radiation safety, was performed by NSLS-II staff. The SPP, PMP and PUA agreements documented the division of NYX responsibilities between NYSBC and NSLS-II. By these agreements, NSLS-II was fully responsible for the initial undulator and straight section and for the Personnel Protection System (PPS), NYSBC engages NSLS-II through the SPP agreement for management activities and to implement the front end, electrical and mechanical utilities, and aspects of the Equipment Protection System (EPS). NYSBC had full responsibility for all other elements. The entire project was coordinated by the BDG partnership.

The NYX project was completed within the period of support and its verification was made with an Instrument Readiness Review (IRR) conducted by NSLS-II to verify readiness to begin technical commissioning. This was a review of all components from source to end station with particular emphasis on radiation safety. The IRR was conducted during 8-9 November 2016 and approval for technical commissioning was granted, which then ensued at the next opportunity on 27 November 2016. These tests proved our novel monochromator concept to be valid and a Comprehensive Radiation Survey that was completed the next day gave us authorization to operate NYX at ring currents up to 300 mA.

The Defense Threat Reduction Agency (DTRA) funding through the Army Research Office (ARO) was used to support the NSLS-II staff engaged in completion of the NYX beamline, for design efforts contracted to Advanced Energy Systems (AES), for front

end components through the SPP arrangement, for utilities and EPS components through the SPP arrangement, and for beam delivery components including the cryocooler (originally contracted to Bruker-ASC and presently Research Instruments GmbH, a majority-owned subsidiary of Bruker Energy & Supercon Technologies, Inc.) and shielding for the white-beam transport. In addition, we have developed the mechanical design for a novel segmented adaptable gap undulator (SAGU) for future implementation to provide enhanced performance.