Responses to Request for Information for DOE-BES Triennial Review of NSLS-II

June 2017

Volume 2a: Beamlines

Specifications, Funding & Productivity

Volume 2a

June 20-21, 2017

Our responses to the questions for the 2017 review are presented in five volumes.

Volume 1 contains general responses to the questions about the facility including budget information, response to recommendations, the organizational structure, development milestones, R&D, and facility input.

Volume 2a contains detailed lists of beamline information (including specifications, funding, publications, and invited talks) as well as the BES surveys for FY15-16, and other supplementary material.

Volume 2b contains the NSLS-II Operations funded Beamline Capability Build-up: Plan and Execution Status.

Volume 3 contains all other requested information and documentation pertinent to this review including support facilities, the user program, and future plans.

Volume 4 is the NSLS-II 2017 5-year Strategic Plan.

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ACRONYMS

ABBIX – Advanced Beamline for Biological
AC-LEEM III – Aberration-Corrected Low Energy Electron Microscope
ACS – American Chemical Society
AMX – Highly Automated Macromolecular Crystallography Beamline
AP-PES – Ambient Pressure Photoelectron Spectroscopy
BER – Biological and Environmental Research
BES – Basic Energy Science
BM – Bending Magnet
BMM – Beamline Materials Measurement
BNL – Brookhaven National Laboratory
CCD – Change Coupled Device
CDW – Collimator Dispersing Wavelength
CHX – Coherent Hard X-ray Scattering
CIF – Crystallographic Information File
CMOS – Complementary Metal Oxide Semiconductor
CMS – Complex Materials Scattering
CPU – Central Processing Unit
CSS – Control System Studio
CSX-1 – Coherent Soft X-ray Scattering
CSX-2 – Soft X-ray Spectroscopy and Polarization
CT – Computed Tomography
DAFS – Diffraction Anomalous Fine Structure
DCM – Double Crystal Monochromator
DLM – Double Laue Monochromator
DMM – Double Multilayer Monochromator
DOE – Department of Energy
EPICS – Experimental Physics and Industrial Control
EPU – Elliptically Polarized Undulator
ESM – Electron Spectro-Microscopy
EXAFS – Extended X-Ray Absorption Fine Structure
FIS – Frontier Synchrotron Infrared Spectroscopy
FMX – Frontier Microfocusing Macromolecular Crystallography
FOE – First Optical Enclosure
FTE – Full Time Equivalent
FTIR – Fourier-Transform Infrared
FXI – Full Field X-ray Imaging
FY – Fiscal Year
FZP – Fresnel Zone Plate
GISAXS – Small Angle X-ray Scattering
GIWAXS – Wide Angle X-ray Scattering
GPU – Graphized Processing Unit
HDM – Horizontally Deflecting Mirror
HRM – Harmonic Rejection Mirror
HXN – Hard X-ray Nanoprobe
ID – Insertion Device
IEEE – Institute of Electrical and Electrician Engineers
IOC – Input/Output Controller
IO-XAS – In Situ and Operando X-ray Absorption Spectroscopy
ISR – Integrated In-Situ and Resonant Hard X-Ray Studies
ISS – Inner-Shell Spectroscopy
IXS – Inelastic X-ray Scattering
KB – Kirkpatrick-Baez
LIX – Life Science X-ray Scattering
MAIA – not an acronym- should be removed
MET – Magnetospectroscopy, Ellipsometry and Time-Resolved Optical Spectroscopies
meV – Milli-Electron Volt
MLL – Multilayer Laue Lens
MOF – Metal Oxide Framework
MX – Macromolecular Crystallography
NEXAFS – Near Edge X-ray Absorption Fine Structure
NEXT – NSLS-II Experimental Tools
NIH – National Institutes of Health
NSLS-II – National Synchrotron Light Source II
NYSDS – New York Scientific Data
NYX – Biological Microdiffraction Facility
PDF – Pair Distribution Function
PFY – Partial Fluoresence yield
PGM – Plane Grating Monochromator
QAS – Quick X-ray Absorption and Scattering
QXRD – Quick X-ray Diffraction
ROI – Region of Interest
SAXS – Small Angle X-ray Scattering
SBM – Side Bounce Monochromator
SIX – Soft Inelastic X-ray Scattering
SMI – Soft Matter Interfaces
SNR – Signal-to-Noise Ratio
SP-ARPES – Spin Polarized Angle Resolution Photon Emission Spectroscopy
SRX – Submicron Resolution X-ray Spectroscopy
SSA – Secondary Source Aperture
SST-1 – Spectroscopy and Tender
SST-2 – Spectroscopy and Tender
SUNY – State University of New York
TES – Tender Energy X-ray Absorption Spectroscopy
TEY – Total Electron Yield
TXM – Transmission X-ray Microscope
UHV – Ultrahigh Vacuum
UV – Ultra Violet
VLS – Variable Line Spacing
WAXS – Wide-Angle X-ray Scattering
XAFS – X-ray Absorption Fire Studies
XANES – X-ray Absorption Near Edge Structure
XAS – X-ray Absorption Spectroscopy
XFM – X-ray Fluorescence Microprobe
XFP – X-ray Footprinting
XPCS – X-ray Photon Correlation Spectroscopy

XPD – X-ray Powder Diffraction
XPEEM – X-ray Photon Electron
XPS – X-ray Photoelectron Spectroscopy
XRD – X-ray Diffraction
ZP – Zone Plate

2.i: Drawing of the floorplan with beamline labels

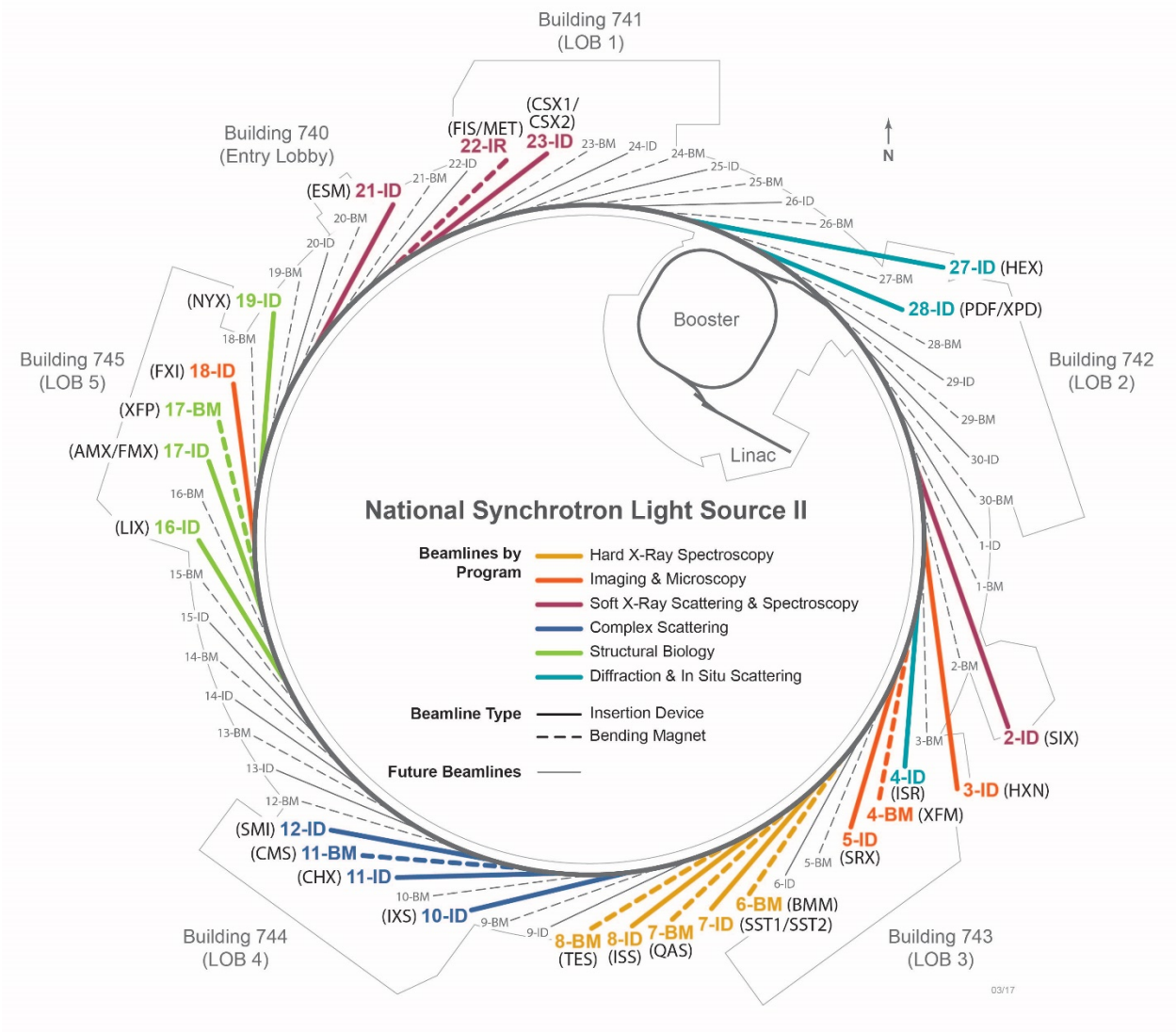

Figure 2.i.1: NSLS II Floorplan

Figure 2.i.1 above shows the floorplan of the facility with the beamlines that are either in operation or are currently under development. The sector number is given for each, along with whether it is a straight sector (ID) or a bending magnet (BM) source or three-pole wiggler. The three-letter name for the beamline is also shown. The color-coding of the beamlines indicates which program the beamline belongs to in the NSLS-II organizational structure. In cases where two beamlines share a single sector they are denoted by a "/" ie. CSX-1/CSX-2. This indicates both beamlines can run independently and simultaneously.

2.ii: Beamline Summary Table

The table below summarizes staffing levels, funding sources, beamtime allocations, unique users and publications of beamlines. This table is reproduced as a pdf on the review website for readability.

NSLS-II Beamline Summary Table

								Staffing (Annually FTEs)														Funding for Operation (Excluded FTE Costs, k$)						Beamtime Allocation (%)								Unique Users								Journal Publications					
								BES funded (FY2016/FY2017 Projected)								Other funded (FY2016/FY2017 Projected)						Annually Funding (FY2017 Projected)		FY2015		FY2016		FY2015				FY2016				FY2015				FY2016				CY2015				CY2016		
								Scientists*		Engineers		Technicians		Others		Scientists		Engineers		Technicians		BES	Others	BES	Others	BES	Others	Maintenance & Start up	User Time			Maintenance & Start up	User Time			General User	Partner User	Facility Staff	Total	General User	Partner User	Facility Staff	Total	Total	with Facility Staff as co-author	High Impact	Total	with Facility Staff as co-author	High Impact
								FY16	FY17 projected	FY16	FY17 projected	FY16	FY17 projected	FY16	FY17 projected	FY16	FY17 projected	FY16	FY17 projected	FY16	FY17 projected								General User	Partner User	Facility Staff		General User	Partner User	Facility Staff															
2-ID	SIX	ID	NSLS-II	P,M	Resonant Inelastic X-ray Scattering	1	BES		1.23	0.13	1.04	0.1	0.57		0.04								233				79.6																							
3-ID	HXN	ID	NSLS-II	M,G,P,A	Scanning X-ray Microscopy (fluorescence, differential phase contrast, diffraction, ptychography	1	BES	2.98	3.2	2.02	1.76	1.74	0.63	0.49	0.605	1*	2*						269		416		507		94.5	5.5	0	0	45.8	49.6	0	4.6	3	0	8	11	53	0	10	63	1	1	0	6	5	1
4-ID	ISR	ID	NSLS-II	M	Real-time GISAXS and GID, RXS, CTR, XMCD	1	BES	0.2	2.53	0.03	1.24	0.02	0.77	0.07	0.09								204				14.7																0	0	5	5						
4-BM	XFM	BM	NSLS-II	G	XRF imaging and tomography, XAFS, XRD	1	BES		0.1				0.1										62				1.2																							
5-ID	SRX	ID	NSLS-II	G,M	XRF imaging, XANES, tomography	1	BES	3.17	2.85	0.98	1.32	1.04	0.53	0.07	0.09			0.35	0.35	0.15	0.15			258		225		258		79.9	20.1	0	0	46.8	50.5	0	2.7	14	0	6	20	105	0	7	112	0	0	0	4	2	1
6-BM	BMM	BM	NIST	M	XAFS, diffraction and DAFS		NIST				0.06				0.05								0.9																												
7-ID-1	SST-1	ID	NIST	M	NEXAFS, NEXAFS Imaging, XPS, XPS Imaging		NIST																																												
7-ID-2	SST-2	ID	NIST	M	NEXAFS, NEXAFS Imaging, XPS, HAXPES, XPS Imaging		NIST																																												
7-BM	QAS	BM	NSLS-II	C,M	Quick and slow XAS and XRD	1	BES		0.1				0.1										11				1																							
8-ID	ISS	ID	NSLS-II	M,C	XAS, XANES, XES, XELS	1	BES	0.24	1.63	0.53	1.55	0.05	0.93	0.07	0.09								296				18.4						91	9	0	0					11	0	4	15				1	0	1
8-BM	TES	BM	NSLS-II	C,G	X-ray absorption spectroscopy, X-ray fluorescence imaging	1	BES		0.71		1.63		0.75		0.09								145				2														1	0	2	3				0	0	0
10-ID	IXS	ID	NSLS-II	P	Ultrahigh resolution inelastic x-ray scattering	1	BES	3.38	3.19	1.43	1.04	0.99	0.5	0.07	0.61	1*	1*						207		416		198		100	0	0	0	56.4	40.2	0	3.4	0	0	7	7	15	0	7	22	0	0	0	0	0	0
11-ID	CHX	ID	NSLS-II	M,P	XPCS, SAXS, GI-SAXS, WAXS	1	BES	2.28	2.18	2.27	2.05	2.11	0.61	0.07	0.09								158		714		431		95.5	4.5	0	0	40.3	55.6	0	4.1	8	0	5	13	32	0	5	37	0	0	0	2	1	0
11-BM	CMS	BM	NSLS-II	M	SAXS/WAXS, GISAXS/GIWAXS	1	BES		1.62		1.07		0.71		0.09								166				23.8														0	1	4	5						
12-ID	SMI	ID	NSLS-II	M,P	X-ray Scattering: GISAXS; GIWAXS, Liquid Reflectivity	1	BES		2.31		1.04		0.71	0.07	0.08								238				23.6																							
16-ID	LIX	ID	NSLS-II	L	Solution scattering; simultaneous SAXS/WAXS; GI-SAXS; microdiffraction	1	NIH/BER				0.35				0.33	2.05	2	2.84	2.95	0.55	1.5	0.04	0.13	5										97.9	1.3	0	0.8					6	0	6	12				0	0	0
17-ID-1	AMX	ID	NSLS-II	L	Macromolecular Crystallography	1	NIH/BER				0.35				0.33	2.05	2	2.84	2.95	0.55	1.5	0.04	0.13	5										99.4	0.6	0	0					3	0	11	14				0	0	0
17-ID-2	FMX	ID	NSLS-II	L	Macromolecular Crystallography, micro-diffraction	1	NIH/BER				0.35				0.33	2.05	2	2.84	2.95	0.55	1.5	0.04	0.13	5										99.4	0.6	0	0					12	0	11	23				0	0	0
17-BM	XFP	BM	CWRU	L	X-ray Footprinting		CWRU				0.35				0.33									5																		3	0	8	11				0	0	0
18-ID	FXI	ID	NSLS-II	M,P	Transmission X-ray Microscopy	1	BES																																												
19-ID	NYX	ID	NYSBC	L	Macromolecular Crystallography		NYSBC				0.17				0.16									2.5																											
21-ID	ESM	ID	NSLS-II	P	ARPES, SP-ARPES, m-ARPES (XPEEM)	1	BES	0.33	2.38	0.13	1.47	0.05	0.93	0.07	0.09								200				8														0	0	4	4						
22-IR	FIS/MET	BM	NSLS-II	P	Spectroscopy, ellipsometery	1	BES																																												
23-ID-1	CSX-1	ID	NSLS-II	M,P	XPCS , Scanning Microscopy, CDI	1	BES	1.74	2.9	1.93	1.89	0.66	0.51	0.21	0.09								263		412		364		84.9	15.1	0	0	39	49.1	7.4	4.5	11	0	5	16	32	9	5	46	1	1	0	2	2	1
23-ID-2	CSX-2	ID	NSLS-II	P,C,M	XAS, XPS, ambient pressure XPS	1	BES	1.27	2	1.65	1.82	0.6	0.45	0.14	0.09	0.35**	0.5+0.35**						201		340		277		100	0	0	0	46.7	33.6	15.6	4.1	0	1	6	7	40	8	7	55	0	0	0	2	2	0
28-ID-1	PDF	ID	NSLS-II	A,C,G,M,P	Time resolved Pair Distribution Function a-lysis (PDF) under varies sample environments; Medium/Wide Angle X-ray Scattering (MAXS-WAXS); Small Angle X-ray Scattering (SAXS)	1	BES																																												
28-ID-2	XPD	ID	NSLS-II	A,M,C,G	high flux or high resolution X-ray Powder Diffraction (XPD); Pair Distribution Function a-lysis (PDF); Tomography and diffraction imaging; Modulation Enhanced XPD	1	BES	3.1	1.79	1.38	1.57	0.97	0.82	0.07	0.09			0.15	0.15					193		382		190		79.7	17	3.3	0	42.3	51.7	3.8	2.2	33	0	4	37	94	11	4	109	5	5	0	21	9	1

Source Type:
Bending Magnet (BM) or Insertion Device (ID)

Area of Research:
A: Applied Sciences
C: Chemical Sciences
G: Geosciences and Environmental Sciences
L: Life Sciences
M: Materials Sciences
P: Physical Sciences

Notes:
Partner contributions omitted if partner user agreement is being revised
Scientists*
Scientists*: LDRD funded unless noted
Scientists**: 0.35 FTE from CFN

Table 2.ii.1: Beamline Summary Table. This table is also published on the review website for readability. In the above table we document, for each beamline, a brief description of the beamline, beamline specifications, names of beamline personnel, and their FTE percentages allocated to each beamline, funding sources and operational funds, allocation percentages, users and publications.

2.iii: Beamlines:

In this section we detail each of the beamlines in operations or under development. The information in this section is the same as in the summary table 2.ii.1 with the exception of the publications. Below we list all publications associated with beamline personnel and the beamline, not just those that utilize NSLS-II photons.

2-ID Soft Inelastic X-ray Scattering (SIX)

Beamline Status

Commissioning

Overall Description

Scientific Scope

Condensed matter physics, material science.

Beamline Description

The SIX beamline will allow resonant inelastic x-ray scattering studies of electronic excitations with ultrahigh energy resolution and continuous momentum tunability. The energy range is 165 to 2300 eV, with linear vertical and circular polarizations available down to 275 eV, and linear horizontal polarization available down to 165 eV. Four energy resolution modes will be made available, medium (90 meV at 1 keV), medium-high (50 meV at 1 keV), high (30 meV at 1 keV), and ultrahigh (14 meV at 1keV). The angle of the spectrometer arm with respect to the incident beam will be tunable between 30 and 150 degrees.

Optical System

A plane, internally cooled mirror (M1) deflects the beam horizontally to the PGM, which consists of an internally cooled plane pre-mirror (M2) and a set of three VLS gratings. The gratings disperse and focus the beam vertically onto the exit slit. A horizontally focusing mirror (M3), with an elliptical figure, focuses the beam horizontally onto the exit slit. An ellipsoidal mirror (M4) is used to focus the secondary source from the exit slit onto the sample spot. The spectrometer consists of two optical branches mirroring each other to double the throughput. Each branch consists of a horizontally collimating parabolic mirror (M5), a vertical focusing mirror (M6) with a circular cylindrical figure, a vertically deflecting plane mirror (M7), a set of two VLS gratings, and a CCD. The optical scheme of the spectrometer relies on the Hettrick-Underwood scheme.

Experimental Apparatus

Sample diffractometer with 6 degrees of freedom, coupled to a cryostat for cooling.

Computer System

Python/EPICS based beamline controls and data acquisition.

Current Capabilities Available for Users (as of 1 May 2017)

N/A

Beamline Specifications

Source Type	Energy Range	Wavelength range	Flux	Focused beam size	Resolution	Technical Quality Metric
EPU57	165-2300 eV	5.39-75.14 Å	≈ 1.5×10^{11} p/s @ 10^{-5} res'n, 8×10^{12} p/s @ 10^{-4} res'n	0.3 x 2.5 μm^2	10^{-4} - 10^{-5}	1

Names of Beamline Personnel and Fractional* FTEs in FY2016

SIX Operations		
WILLIAM	OBRIEN	0.06
MICHAEL	BROMFIELD	0.05
8 other staff members contributed effort		0.12
Total		0.23

*Note: 1.0 FTE based on 1760 hours of work. Some staff may log more hours annually

Funding source and fraction of funding for each source FY15-16

FY 2015: DOE – BES; 100%
FY 2016: DOE – BES; 100%
FY 2017: DOE – BES; 100%

Operating funds FY15-16 (K$)

Fiscal Year	Labor Costs	Contract Milestone Payments	Travel	Contract Labor, JT Appts & Shops	Maint/Svc Contracts	Materials & Purchasing	Total Cost
2015	n/a	n/a	n/a	n/a	n/a	n/a	n/a
2016	52K	1K	6K	73K		1 k	132K

Allocation Percentages

Fiscal Year**	Maintenance & Start up	General Users	Partner Users	Facility Staff
2015	n/a	n/a	n/a	n/a
2016	n/a	n/a	n/a	n/a
2017	100	0	0	0

** Partial year for 2017.

Number of unique beamline users each year

Fiscal Year**	General Users	Partner Users	Facility Staff	Total
2015	n/a	n/a	n/a	n/a
2016	n/a	n/a	n/a	n/a
2017	0	0	9	9

** Partial year for 2017.

Publications: (all publications used NSLS-II photons; numbers in parentheses indicates staff co-authorship)

Calendar Year**	Refereed	DOE High Profile	DOE High Impact	All Publications
2015	n/a	n/a	n/a	n/a
2016	n/a	n/a	n/a	n/a
2017	n/a	n/a	n/a	n/a

** Partial year for 2017.

Complete List of Publications for CY15-17

(includes publications that used NSLS-II photons, beamline R&D publications by staff, and staff research publications; red text indicates publications that used NSLS-II photons)

Refereed Journal Publications

- D Meyers, H Miao, A Walters, V Bisogni, R Springell, M d'Astuto, M Dantz, J Pelliciari, H Huang, et al., Doping Dependence of the Magnetic Excitations in La 2−x Sr x CuO 4, Phys. Rev. B: Condens. Matter, 95, 075139 (2017).
- S Johnston, C Monney, V Bisogni, K Zhou, R Kraus, G Behr, V Strocov, J Malek, S Drechsler, et al., Electron-lattice Interactions Strongly Renormalize the Charge-transfer Energy in the Spin-chain Cuprate Li2CuO2 , Nat. Commun., 7, 10653 (2016). [112581]
- J Pelliciari, Y Huang, T Das, M Dantz, V Bisogni, P Olalde Velasco, V Strocov, L Xiang, X Wang, et al., Intralayer Doping Effects on the High-energy Magnetic Correlations in NaFeAs, Phys. Rev. B: Condens. Matter, 93, 134515 (2016). [112579]

- V Bisogni, S Catalano, R Green, M Gibert, R Scherwitzl, Y Huag, V Stgrocov, P Zubko, S Balandeh, et al., Ground-state Oxygen Holes and the Metal–insulator Transition in the Negative Charge-transfer Rare-earth Nickelates, Nat. Commun., 7, 13017 (2016).
- C Monney, V Bisogni, K Zhou, R Kraus, V Strocov, G Behr, S Drechsler, H Rosner, S Johnston, et al., Probing Inter- and Intrachain Zhang-Rice Excitons in Li2CuO2 and Determining their Binding Energy, Phys. Rev. B: Condens. Matter, 94(16), 165118 (2016).
- J Hancock, I Jarrige, The Promise of Resonant Inelastic X-ray Scattering for Modern Kondo Physics, J. Magn. Magn. Mater., 400, 41-46 (2016).
- T Nomura, Y Harada, H Niwa, K Ishii, M Ishikado, S Shamoto, I Jarrige, Resonant Inelastic X-ray Scattering Study of Entangled Spin-orbital Excitations in Superconducting PrFeAsO0.7, Phys. Rev. B: Condens. Matter, 94, 035134 (2016).
- J Dvorak, I Jarrige, V Bisogni, S Coburn, W Leonhardt, Towards 10 meV Resolution: The Design of an Ultrahigh Resolution Soft X-ray RIXS Spectrometer, Rev. Sci. Instrum., 87(11), 115109 (2016).
- M Yoshida, K Ishii, M Naka, S Ishihara, I Jarrige, K Ikeuchi, Y Murakami, K Kudo, Y Koike, et al., Observation of Momentum-resolved Charge Fluctuations Proximate to the Charge-order Phase Using Resonant Inelastic X-ray Scattering, Sci. Rep., 6, 23611 (2016).
- V Bisogni, K Wohlfeld, S Nishimoto, C Monney, J Trinckauf, K Zhou, R Kraus, K Koepernik, C Sekar, et al., Orbital Control of Effective Dimensionality: From Spin-Orbital Fractionalization to Confinement in the Anisotropic Ladder System CaCu2O3, Phys. Rev. Lett., 114(9), 096402 (2015).
- S Catalano, M Gibert, V Bisogni, F He, R Sutarto, M Viret, P Zubko, R Scherwitzl, G Sawatzky, et al., Tailoring the Electronic Transitions of NdNiO3 Films Through (111)pc Oriented Interfaces, APL Mater., 3, 062506 (2015).
- I Jarrige, K Ishii, D Matsumura, Y Nishihata, M Yoshida, H Kishi, M Taniguchi, M Uenishi, H Tanaka, et al., Toward Optimizing the Performance of Self-Regenerating Pt-Based Perovskite Catalysts, ACS Catal., 5(2), 1112-1118 (2015).
- L Wray, S Huang, I Jarrige, K Ikeuchi, K Ishii, J Li, Z Qiu, Z Hussain, Y Chuang, Extending Resonant Inelastic X-ray Scattering to the Extreme Ultraviolet, Front. Phys., 3, 32-1 (2015).
- H Yamaoka, E Schwier, M Arita, K Shaimada, N Tsujii, I Jarrige, J Jiang, H Hayashi, H Iwasawa, et al., Electronic Structure of the Heavy-fermion Caged Compound Ce3Pd20X6 (X = Si, Ge) Studied by Density Functional Theory and Photoelectron Spectroscopy, Phys. Rev. B: Condens. Matter, 91, 115139 (2015).
- I Jarrige, A Kotani, H Yamoaka, N Tsujii, K Ishii, M Upton, D Casa, J Kim, T Gog, J Hancock, Kondo Interactions from Band Reconstruction in YbInCu4, Phys. Rev. Lett., 114, 126401 (2015).
- H Gretarsson, T Nomura, I Jarrige, A Lupascu, M Upton, J Kim, D Casa, T Gog, R Yuan, et al., Resonant inelastic X-ray Scattering Study of Electronic Excitations in Insulating K0.83Fe1.53Se2, Phys. Rev. B: Condens. Matter, 91, 245118 (2015).

3-ID Hard X-ray Nano-probe (HXN)

Beamline Status

Operations

Overall Description

Scientific Scope

Hard x-ray nanoprobe (HXN) is an undulator beamline at sector 3-ID providing x-ray imaging capabilities with a world-leading spatial resolution. It offers a suite of x-ray analytical tools for structural, elemental and chemical imaging, with an initial resolution of 10 nm and an ultimate goal of 1 nm. The combination of unique detection capabilities of x-rays and the unprecedented resolution enables noninvasive material characterizations at nanometer scale, critical for studies in many areas of science and technology.

Beamline Description

The Hard X-ray Nanoprobe (HXN) is an undulator beamline at sector 3-ID providing structural and X-ray fluorescence imaging with world-leading spatial resolution. The scientific mission of the beamline is to enable hard X-ray imaging of structure, elements, strain and chemical states with spatial resolutions ranging from 10 to 30 nm with an ultimate goal of ~1 nm.

Optical System

Major components of the beamline optical system include a horizontal collimating mirror, a horizontal double-crystal monochromator, a horizontal focusing mirror, a set of vertical focusing compound-refractive lenses and two secondary source apertures.

Experimental Apparatus

Major apparatus include a MLL module for 10 nm resolution, a FZP module for 30 nm resolution, rotation stages for tomography, and heating and cooling stages.

Computer System

Workstations, CPU and GPU clusters and data analysis software.

Current Capabilities Available for Users (as of 1 May 2017)

- 2D Scanning X-ray fluorescence imaging with a minimum beam size of 15 nm with an energy range of 12-16 keV (using multilayer Laue lenses).
- 2D and 3D scanning X-ray fluorescence imaging with a minimum beam size of 60 nm with an energy range of 6-12 keV (using a zone plate).

- 2D XANES imaging with a minimum beam size of 60 nm with an energy range of 6-12 keV (using a zone plate).
- 2D Scanning X-ray Bragg diffraction imaging (i.e. nanodiffraction) with a minimum beam size of 60 nm with an energy range of 8-12 keV (using a zone plate). The measurement is limited to a single reflection from single crystalline sample with a well-defined crystal orientation.
- Transmission X-ray ptychography with an energy range of 8-16 keV.
- Bragg CDI/Ptychography on single crystal samples. Strong emphasis is on developing analysis software.
- Multimodality 3D imaging with higher resolutions.

Beamline Specifications

Source Type	Energy Range	Wavelength range	Flux	Focused beam size	Resolution	Technical Quality Metric
IVU20	6-25 KeV	λ=2.07-0.50 Å	≈ 5 x 10^8 p/s (@10KeV)	10 nm (MLL) ~30 nm (ZP)	dE/E ~ 10^{-4}	1

Names of Beamline Personnel and Fractional* FTEs in FY2016

HXN Operations		
XIAOJING	HUANG	1.05
YONG	CHU	1.00
HANFEI	YAN	0.80
PETR	ILINSKI	0.78
JAMES	BIANCAROSA	0.49
MIKE	MAKLARY	0.46
WEIHE	XU	0.41
SEBASTIAN	KALBFLEISCH	0.27
DENNIS	KUHNE	0.17
ANDREW	DESANTIS	0.15
LUKAS	LIENHARD	0.15
WEN	HU	0.10
PAUL	PALECEKJR	0.10
MARY	CARLUCCIDAYTON	0.09
HARMANPREET	BASSAN	0.07
SUSAN	MALDONADO	0.07
ROBERT	TODD	0.05
50 other staff members contributed effort		1.02
Total		7.22

*Note: 1.0 FTE based on 1760 hours of work. Some staff may log more hours annually

Funding source and fraction of funding for each source FY15-16

FY 2015: DOE – BES; 100%
FY 2016: DOE – BES; 100%
FY 2017: DOE – BES; 100%

Operating funds FY15-16 (K$)

Fiscal Year	Labor Costs	Contract Milestone Payments	Travel	Contract Labor, JT Appts & Shops	Maint/Svc Contracts	Materials & Purchasing	Total Cost
2015	1,767K	0	17K	128K	12K	259K	2,183K
2016	1,737K	0	50K	22K	46K	388K	2,244K

Allocation Percentages

Fiscal Year**	Maintenance & Start up	General Users	Partner Users	Facility Staff
2015	94.5	5.5	0	0
2016	45.8	49.6	0	4.6
2017	28	67	0	5

** Partial year for 2017.

Number of unique beamline users each year

Fiscal Year**	General Users	Partner Users	Facility Staff	Total
2015	3	0	8	11
2016	53	0	10	63
2017	48	0	8	56

** Partial year for 2017.

Publications: (all publications used NSLS-II photons; numbers in parentheses indicates staff co-authorship)

Calendar Year**	Refereed	DOE High Profile	DOE High Impact	All Publications
2015	0 (0)	0 (0)	0 (0)	1 (1)
2016	6 (5)	0 (0)	1 (1)	6 (5)
2017	1 (0)	0 (0)	0 (0)	1 (0)

** Partial year for 2017.

Complete List of Publications for CY15-17

(includes publications that used NSLS-II photons, beamline R&D publications by staff, and staff research publications; red text indicates publications that used NSLS-II photons)

- H Feng, Y Qian, J Cochran, Q Zhu, W Hu, H Yan, L Li, X Huang, Y Chu, et al., Nanoscale Measurement of Trace Element Distributions in Spartina Alterniflora Root Tissue During Dormancy, Sci. Rep., 7, 40420 (2017).
- I Robinson, X Huang, X-ray Imaging: Reaching the Third Dimension, Nat. Mater., 16, 160–161 (2017).
- X Huang, W Xu, E Nazaretski, N Bouet, J Zhou, Y Chu, H Yan, Hard X-ray Scanning Imaging Achieved with Bonded Multilayer Laue Lenses, Opt. Express, 25(8), 8698-8704 (2017).
- Z Zhang, Q Zhang, J Shi, Y Chu, X Yu, K Xu, M Ge, H Yan, W Li, et al., A Self-Forming Composite Electrolyte for Solid-State Sodium Battery with Ultralong Cycle Life, Adv. Energy Mater., 7(4), 1601196 (2016).
- E Nazaretski, W Xu, N Bouet, J Zhou, H Yan, X Huang, Y Chu, Development and Characterization of Monolithic Multilayer Laue Lens Nanofocusing Optics, Appl. Phys. Lett., 108, 261102 (2016).
- J Weker, X Huang, M Toney, In Situ X-ray-based Imaging of Nano Materials, Current Opinion in Chemical Engineering 12, 14-21 (2016).
- H Yan, E Nazaretski, K Lauer, X Huang, U Wagner, C Rau, M Yusuf, I Robinson, S Kalbfleisch, et al., Multimodality Hard-x-ray Imaging of a Chromosome with Nanoscale Spatial Resolution, Sci. Rep., 6, 20112 (2016).
- H Ozturk, H Yan, J Hill, Correlating Sampling and Intensity Statistics in Nanoparticle Diffraction Experiments, J. Appl. Cryst., 48(4), 1212-1227 (2015).
- E Nazaretski, K Lauer, H Yan, N Bouet, J Zhou, R Conley, X Huang, W Xu, M Lu, et al., Pushing the Limits: An Instrument for Hard X-ray Imaging Below 20 nm, J. Synch. Rad., 22(2), 336-341 (2015).
- B Collins, Y Chu, L He, D Haskel, F Tsui, Structural and Chemical Ordering of Heusler Co_xMn_yGe_z Epitaxial Films on Ge (111): Qunatitative Study Using Tranditional and Anomalous x-ray Diffraction Techniques, Phys. Rev. B: Condens. Matter, 92, 224108 (2015).
- C Zhu, R Harder, A Diaz, V Komanicky, A Barbour, R Xu, X Huang, Y Liu, M Pierce, et al., Ptychographic X-ray Imaging of Surfaces on Crystal Truncation Rod, Appl. Phys. Lett., 106(10), 101604 (2015).
- J Kim, N Habekorn, E Nazaretski, R da Paula, T Tan, X Xi, T Tajima, R Movshovich, L Civale, Strong Magnetic Field Dependence of Critical Current Densities and Vortex Activation Energies in Ananisotropic Clean MgB2 Thin Film, Solid State Commun., 204, 56-60 (2015).
- X Huang, R Conley, N Bouet, J Zhou, A Macrander, J Maser, H Yan, E Nazaretski, K Lauer, et sl., Achieving Hard X-ray Nanofocusing Using a Wedged Multilayer Laue Lens, Opt. Express, 23(10), 12496-12507 (2015).
- N Burdet, X Shi, D Park, J Clark, X Huang, S Kevan, I Robinson, Evaluation of partial coherence correction in X-ray ptychography, Opt. Express, 23(5), 5452-5467 (2015).
- X Huang, K Lauer, J Clark, W Xu, E Evgeny, R Harder, I Robinson, Y Chu, Fly-scan Ptychography, Sci. Rep., 5, 9074 (2015).
- X Huang, W Yang, R Harder, Y Sun, M Lu, Y Chu, I Robinson, H Mao, Deformation Twinning of a Silver Nanocrystal under High Pressure, Nano Lett., 15(11), 7644-7649 (2015).

Refereed Conference Proceedings

- E Nazaretski, H Yan, K Lauer, X Huang, S Kalbfleisch, H Yan, L Li, N Bouet, J Zhou, et al., Nm-scale Spatial Resolution X-ray Imaging with MLL Nanofocusing Optics: Instrumentational Requirements and Challenges, ICXOM23: International Conference on X-ray Optics and Microanalysis, sponsored by DOE (2016).
- J Fitts, A Lanzirotti, A Acerbo, Y Chu, B Dazas, X Huang, E Nazaretski, G Rogers, R Tappero, et al., Salinity Effects on Arsenic Incorporation During Barite Precipitation Treatment of Idealized Shale Gas Wastewaters, American Chemical Society National Meeting & Exposition, Vol 252, sponsored by American Chemical Society (2016).
- A Lanzirotti, S Sutton, M Newville, J Fitts, E Head, High Energy Synchrotron X-ray Microspectroscopy for Geochemical Characterization of Terrestrial and Extraterrestrial Samples, Geological Society of America Annual Meeting, Vol 48, p. 35-2, sponsored by Geological Society of America (2016).
- O Chubar, Y Chu, X Huang, S Kalbfleisch, H Yan, T Shaftan, G Wang, Y Qai, Y Chen-Wiegart, et al., Initial Performances of First Undulator-based Hard X-ray Beamlines of NSLS-II Compared to Simulations, AIP Conference Proceedings, Vol 1741, p. 040002, sponsored by AIP Conf. Proc. (2016).
- Y Chu, H Yan, E Nazaretski, S Kalbfleisch, X Huang, K Lauer, N Bouet, Hard x-ray nanoprobe Facility at the National Synchrotron Light Source II, SPIE prepared for SPIE (2015).
- J Clark, M Trigo, T Henighan, R Harder, B Abbey, T Katayama, M Kozina, E Dufresne, H Wen, et al., Lensless Imaging of Nano- and Meso-Scale Dynamics with X-rays, Microscopy and Microanalysis, Vol 21, p. 1081, sponsored by Microscopy Society of America (2015).
- W Xu, K Lauer, H Yan, V Milanovic, M Lu, E Nazaretski, Performance and Characterization of a MEMS-based Device for Alignment and Manipulation of X-ray Nanofocusing Optics, AIP Adv., 5, 037137 (2015).

Other Publications (books, theses, etc)

- D Shu, Y Chu, High Precision Detector Robot Arm System, US Patent No. US 9,557,282 B1 (2017).
- R Conley, N Bouet, Y Chu, X Huang, H Kang, A Macrander, J Maser, E Nazaretski, G Stephenson, H Yan, Multilayer Laue Lens: A Brief History and Current Status, Synch. Rad. News, 29(4), 16 (2016).

4-BM X-ray Fluorescence Microprobe (XFM)

Beamline Status

Construction

Overall Description

Scientific Scope

XFM is a versatile X-ray Fluorescence Microscope optimized for spatially-resolved characterization of elemental abundances and chemical speciation in heterogeneous samples.

Beamline Description

XFM is unique as a spectroscopy beamline because it spans the tender (2-5 keV) and hard (5-23keV) energy range (P to Tc K-edges), and also offers a polychromatic "pink" mode ideal for rapid 2D and 3D fluorescence imaging and tomography. It employs compound focusing to achieve a user-tunable spot size from 1 to 10 microns while maintaining a long working distance for physically large samples and custom in situ environmental cells. If desired, a pre-focused bulk (1x1mm) beam is available at the sample position for medium energy powder XRD and bulk EXAFS measurements.

Optical System

Compound focusing: Toroidal macro-focusing mirror illuminates a secondary source aperture (SSA), and a pair of KB micro-focusing mirrors is used to image the secondary source; beam diverging from the SSA is collimated vertically with a bent flat mirror and monochromated with Si(111) or Si(311) crystal pairs.

Experimental Apparatus

Vortex ME4 SDD with Quantum Xspress3 DXPs or Canberra 13-element Germanium Array detector with XIA XMAPS DXPs. MAIA-384 detector with custom FPGA electronics. Rayonix 165 CCD detector or MAR 345 image plate. Ion chambers and photodiode detectors. XYZ-theta high-resolution motorized sample position stages. Motorized experimental tables (5-degrees of freedom). CCD-coupled optical microscopes with epifluorescence capabilities. Peltier cold stage (-20C), Linkham cryostage (-150C), and cryostream sample cooling capabilities.

Computer System

Beamline components are controlled by EPICS 3.14 using VME. The user interface is through the Python and Control System Studio (CSS) clients. The user views the experimental system (sample and the surrounding environment) through CCD-coupled optical microscopes with

Prosilica cameras. Windows 7 workstations running Python and CSS clients; Linux Debian running IOCs and CSS clients.

Current Capabilities Available for Users (as of 1 May 2017)

N/A

Beamline Specifications

Source Type	Energy Range	Wavelength range	Flux	Focused beam size	Resolution	Technical Quality Metric
3PW	2.3-23 KeV		$\approx 10^{11}$ p/s	1 -1000 µm	$\sim 10^{-4}$	

Names of Beamline Personnel and Fractional* FTEs in FY2016

*Note: 1.0 FTE based on 1760 hours of work. Some staff may log more hours annually

Funding source and fraction of funding for each source FY15-16

FY 2015: DOE – BES; 100%
FY 2016: DOE – BES; 100%
FY 2017: DOE – BES; 100%

Operating funds FY15-16 (K$)

Fiscal Year	Labor Costs	Contract Milestone Payments	Travel	Contract Labor, JT Appts & Shops	Maint/Svc Contracts	Materials & Purchasing	Total Cost
2015	n/a	n/a	n/a	n/a	n/a	n/a	n/a
2016	n/a	n/a	n/a	n/a	n/a	n/a	n/a

Allocation Percentages

Fiscal Year**	Maintenance & Start up	General Users	Partner Users	Facility Staff
2015	n/a	n/a	n/a	n/a
2016	n/a	n/a	n/a	n/a
2017	n/a	n/a	n/a	n/a

** Partial year for 2017.

Number of unique beamline users each year

Fiscal Year**	General Users	Partner Users	Facility Staff	Total
2015	n/a	n/a	n/a	n/a
2016	n/a	n/a	n/a	n/a
2017	n/a	n/a	n/a	n/a

** Partial year for 2017.

Publications: (all publications used NSLS-II photons; numbers in parentheses indicates staff co-authorship)

Calendar Year**	Refereed	DOE High Profile	DOE High Impact	All Publications
2015	n/a	n/a	n/a	n/a
2016	n/a	n/a	n/a	n/a
2017	n/a	n/a	n/a	n/a

** Partial year for 2017.

Complete List of Publications for CY15-17

(includes publications that used NSLS-II photons, beamline R&D publications by staff, and staff research publications; red text indicates publications that used NSLS-II photons)

Refereed Journal Publications

- F Ono, R Tappero, D Sparks, L R G Guilherme, Investigation of Arsenic Species in Tailings and Windblown Dust from a Gold Mining Area, Environ. Sci. Pollut. R, 23(1), 638-647 (2016).
- P Allison, J Seiter, A Diaz, J Lindsay, R Moser, R Tappero, A Kennedy, Gastropod (Otala lactea) Shell Nanomechanical and Structural Characterization as a Biomonitoring Tool for Dermal and Dietary Exposure to a Model Metal, J. Mech. Behavior Biomed., 53, 142-150 (2016).
- H Feng, Y Qian, F J Gallagher, W Zhang, L Yu, C J Liu, K W Jones, R Tappero, Synchrotron Micro-scale Measurement of Metal Distributions in Phragmites Australis and Typha Latifolia Root Tissue from an Urban Brownfield Site, 41, 172-182 (2016). [112048]
- S Karuppagounder, I Alim, S Khim, M Bourassa, S Sleiman, R John, C Thinnes, T Yeh, R Tappero, et al., Therapeutic Targeting of Oxygen-sensing Prolyl Hydroxylases Abrogates ATF4-dependent Neuronal Death and Improves Outcomes After Brain Hemorrhage in Several Rodent Models, Sci. Transl. Med., 8(328), 328ra29 (2016). [112574]
- P Northrup, A Leri, R Tappero, Applications of “Tender” Energy (1-5 keV) X-ray Absorption Spectroscopy in Life Sciences, Protein Peptide Lett., 23(3), 300-308 (2016). [112578]
- H Feng, W Zhang, Y Qian, W Liu, L Yu, S Yoo, J Wang, J J Wang, R Tappero, et al., Synchrotron X-ray Microfluorescence Measurement of Metal Distributions in Phragmites australis Root System in the Yangtze River Intertidal Zone, J. Synch. Rad., 23, 937-946 (2016).
- E Stach, Y Li, S Zhao, A Gamalski, D Zakharov, R Tappero, K Chen-Wiegart, J Thieme, U Jung, et al., Characterizing Working Catalysts with Correlated Electron and Photon Probes, Microsc. Microanal., 21, 563-564 (2015).

- C Thompson, J Wolf, R Elbekai, M Paranjpe, J Seiter, M Chappell, R Tappero, M Suh, D Proctor, et al., Duodenal Crypt Health Following Exposure to Cr(VI): Micronucleus Scoring, γ-H2AX Immunostaining, and Synchrotron X-ray Fluorescence Microscopy, 789-790, 61-66 (2015).
- K H Kim, R Tappero, E Bolotinikov, A Hossain, G Yang, R B James, P Fochuk, Long-term Stability of Ammonium-sulfide- and Ammonium-fluoride-passivated CdMnTe Detectors, J. Korean Physical Soc., 66, 1532-1536 (2015).
- U N Roy, A E Bolotnikov, G S Camarda, Y Cui, A Hossain, K Lee, R Tappero, G Yang, A Burger, R B James, Compositional Homogeneity and X-ray Topographic Analyses of CdTexSe1-x Grown by the Vertical Bridgman Technique, J. Cryst. Growth, 411, 34-37 (2015).
- U N Roy, A E Bolotnikov, G S Camarda, Y Cui, A Hossain, W Lee, R Tappero, G Yang, R Gul, R B James, High Compositional Homogeneity of CdTexSe1-x crystals Grown by the Bridgman Method, APL Mater., 3, 026102 (2015).
- H Feng, W Zhang, W Liu, L Yu, Y Qian, J Wang, C Eng, C J Liu, K W Jones, R Tappero, Synchrotron Micro-scale Study of Trace Metal Transport and Distribution in Spartina Alterniflora Root System in Yangtze River intertidal Zone, Environ. Sci. Pollut. R, 22(23), 18933-18944 (2015).
- Qian, H Feng, F Gallagher, Q Zhu, M Wu, C Liu, K Jones, R Tappero, Synchrotron Study of Metal Localization in Typha Latifolia L. Root Sections, J. Synch. Rad., 22(6), 1459-1468 (2015). [112050]
- D E Crean, C L Corkhill, T Nicholls, R Tappero, J M Collins, N C Hyatt, Expanding the Nuclear Forensic Toolkit: Chemical Profiling of Uranium Ore Concentrate Particles by Synchrotron X-ray Microanalysis, RSC Adv., 5, 87908-87918 (2015).
- F B. Ono, E S. Penido, R Tappero, D Sparks, L R. G Guilherme, Bioaccessibility of Cd and Pb in Tailings from a Zinc Smelting in Brazil: Implications for Human Health, Environ. Geochem. Hlth., 38(5), 1083-1096 (2015).
- S Zhao, Y Li, E Stavitski, R Tappero, S Crowley, M J Castaldi, D N Zakharov, R G Nuzzo, A I Frenkel, E A Stach, Operando Characterization of Catalysts with a Portable Microreactor, ChemCatChem, 7(22), 3683-3691 (2015). [108512]
- D Bock, R Tappero, K Takeuchi, A Marschilok, E Takeuchi, Mapping the Anode Surface-Electrolyte Interphase: Investigating a Life Limiting Process of Lithium Primary Batteries, ACS Appl. Mater. Interfaces, 7(9), 5429-5437 (2015). [107807]
- Y Li, D Zakharov, S Zhao, R Tappero, U Jung, A Elsen, P Baumann, R G Nuzzo, E A Stach, A I Frenkel, Complex Structural Dynamics of Nanocatalysts Revealed in Operando Conditions by Correlated Imaging and Spectroscopy Probes, Nat. Commun., 6, 7583 (2015).

Refereed Conference Proceedings

- J Fitts, A Lanzirotti, A Acerbo, Y Chu, B Dazas, X Huang, E Nazaretski, G Rogers, R Tappero, et al., Salinity Effects on Arsenic Incorporation During Barite Precipitation Treatment of Idealized Shale Gas Wastewaters, American Chemical Society National Meeting & Exposition, Vol 252, sponsored by American Chemical Society (2016).
- E Stach, Y Li, S Zhao, A Gamalski, D Zakharov, R Tappero, K Chen-Weigart, J Thieme, R Nuzzo, A Frenkel, Characterizing Working Catalysts with Correlated Electron and Photon Probes, Microscopy and Microanalysis, sponsored by Microscopy Society of America (2015).

4-ID Integrated In-situ and Resonant Hard X-ray Studies (ISR)

Beamline Status

Commissioning

Overall Description

Scientific Scope

The primary goal of the ISR beamline is to illuminate the physics of materials for the 21st century, and the science scope consists of three overlapping areas: novel ordering phenomena, atomic structure of functional surfaces and interfaces, and growth and materials processes.

Beamline Description

ISR supports x-ray scattering techniques (e.g., resonant x-ray scattering, crystal truncation rod measurements, x-ray reflectivity, grazing incidence small-angle x-ray scattering, and grazing incidence diffraction) in order to improve our understanding of novel materials. Specialized optics provide polarization control, and a flexible range of environment chambers can be accommodated for in-situ studies of materials.

Optical System

Si(111) DCM; primary focusing optics to focus at any of three endstations or at the SSA, which is ~50 m from the source; polarization control (circular as well as variable linear); harmonic rejection mirror.

Experimental Apparatus

Three endstations: a horizontal scattering plane base diffractometer, a 6-circle diffractometer, and a base diffractometer that accommodates UHV growth chambers. Displex cryostat; gas handling system; polarization analyzers; point and area detectors, including a Vortex silicon drift detector, a Pilatus 100K, and an Eiger 1M.

Computer System

Linux workstations.

Current Capabilities Available for Users (as of 1 May 2017)

- Single-crystal resonant X-ray scattering with hard X-rays (6-23 keV), ~100 micron beam
- In-situ studies of materials growth at surfaces and interfaces in user-supplied growth chamber with hard X-rays (8-23 keV), optional use of gas flow control and handling capabilities for non-hazardous gases, ~100 micron beam

- Polarization-dependent, single-crystal X-ray scattering with hard X-rays (6-14 kev), ~100 micron beam
- In-situ studies of materials growth at surfaces and interfaces in user-supplied growth chamber with hard X-rays (8-23 keV), ~20 micron beam

Beamline Specifications

Source Type	Energy Range	Wavelength range	Flux	Focused beam size	Resolution	Technical Quality Metric
IVU23	2.4 - 23 KeV	λ=0.54-5.2 Å	≈ 10^{13} p/s	2 x 20 µm2	~ 10^{-4}	1

Names of Beamline Personnel and Fractional* FTEs in FY2016

ISR Operations		
KENNETH	EVANSLUTTERODT	0.11
CHRISTIE	NELSON	0.10
SUSAN	MALDONADO	0.07
7 other staff members contributed effort		0.05
Total		0.32

*Note: 1.0 FTE based on 1760 hours of work. Some staff may log more hours annually

Funding source and fraction of funding for each source FY15-16

FY 2015: DOE – BES; 100%
FY 2016: DOE – BES; 100%
FY 2017: DOE – BES; 100%

Operating funds FY15-16 (K$)

Fiscal Year	Labor Costs	Contract Milestone Payments	Travel	Contract Labor, JT Appts & Shops	Maint/Svc Contracts	Materials & Purchasing	Total Cost
2015	n/a	n/a	n/a	n/a	n/a	n/a	n/a
2016	103K		13K	0 k		3K	119K

Allocation Percentages

Fiscal Year**	Maintenance & Start up	General Users	Partner Users	Facility Staff
2015	n/a	n/a	n/a	n/a
2016	n/a	n/a	n/a	n/a
2017	83.0	15.0	0.0	2.0

** Partial year for 2017.

Number of unique beamline users each year

Fiscal Year**	General Users	Partner Users	Facility Staff	Total
2015	n/a	n/a	n/a	n/a
2016	n/a	n/a	n/a	n/a
2017	8	0	2	10

** Partial year for 2017.

Publications: (all publications used NSLS-II photons; numbers in parentheses indicates staff co-authorship)

Calendar Year**	Refereed	DOE High Profile	DOE High Impact	All Publications
2015	n/a	n/a	n/a	n/a
2016	n/a	n/a	n/a	n/a
2017	0	0	0	0

** Partial year for 2017.

Complete List of Publications for CY15-17

(includes publications that used NSLS-II photons, beamline R&D publications by staff, and staff research publications; red text indicates publications that used NSLS-II photons)

Refereed Journal Publications

- W Miller, L Wu, M Kim, T Orvis, J Simonson, M Gamza, D McNally, C Nelson, G Ehlers, et al., Magnetic Structure of Yb2Pt2Pb: Ising Moments on the Shastry-Sutherland Lattice, Phys. Rev. B: Condens. Matter, 93(10), 104419 (2016).
- T Gupta, A Kim, S Phadke, S Biswas, T Luong, B Hertzberg, M Chamoun, K Evans-Lutterodt, D Steingart, Improving the Cycle Life of a High-rate, High-potential Aqueous Dual ion Battery using Hyper-dendritic Zinc and Copper Hexacyanoferrate, J. Power Sources, 305, 22-29 (2016).
- H Zhang, T Yu, Z Chen, C Nelson, L Bezmaternykh, A Abeykoon, T Tyson, Probing Magnetostructural Correlations in Multiferroic HoAl3(BO3)4, Phys. Rev. B: Condens. Matter, 92, 104108 (2015).

- V Stanic, J Bettini, F E. Montoro, A Stein, K Evans-Lutterodt, Local Structure of Human Hair Spatially Resolved by Sub-micron X-ray Beam, Sci. Rep., 5, 17347 (2015).

5-ID Submicron Resolution X-ray Spectroscopy (SRX)

Beamline Status

Operations

Overall Description

Scientific Scope

Submicron Resolution X-ray Spectroscopy (SRX) is an undulator beamline at sector 5-ID providing world-leading, high-throughput spectroscopic imaging capability (2D and 3D) with sub-100 nm spatial resolution and millisecond dwell times/pixel with fly-scan capability. Scientific communities such as environmental sciences, life sciences, and material sciences will take advantage of this beamline to understand complex natural and engineered systems that are heterogeneous on the micron to nanometer scale.

Beamline Description

The Submicron Resolution X-ray Spectroscopy beamline, SRX, will enable simultaneous x-ray fluorescence and transmission measurements with sub-µm to sub-100 nm spatial resolution with an incident x-ray beam energy of 4.65-25 keV. X-rays are focused onto the sample by a set of Kirkpatrick-Baez mirrors. Sample stages will enable fast 2D scanning and tomography capabilities. X-ray fluorescence imaging and tomography will provide elemental mapping in 2D and 3D, respectively. Spatially resolved X-ray Absorption Near Edge Structure (XANES) spectroscopy can be performed in fluorescence or transmission mode. Full-field imaging and tomography are also possible to provide morphology information. Several different operation modes including high resolution scanning (sub-100 nm focused beam), high flux (sub-µm focused beam) scanning and full-field imaging are available.

Optical System

Horizontally focusing mirror, Horizontal double crystal monochromator, secondary source slits, Kirkpatrick-Baez mirrors (2 sets - high flux and high resolution modes, respectively).

Experimental Apparatus

X-ray fluorescence spectroscopy - Vortex ME3 (Hitachi), MAIA detector (in collaboration wtih Peter Siddons); X-ray absorption near edge structure (XANES) in transmission mode: photodiode (Hamamatsu); full-field imaging/tomography: CMOS (PCO- edge)

Computer System

Beamline control: EPICS, CS-Studio, Python

Current Capabilities Available for Users (as of 1 May 2017)

- X-ray Fluorescence Imaging with a beam size of 1 micron or better
- XANES Spectroscopy with a beam size of 1 micron or better
- EXAFS Spectroscopy with a beam size of 1 micron or better
- X-ray fluorescence microscopy with the 384-element Maia detector and a beam size of 1 micron or better

Beamline Specifications

Source Type	Energy Range	Wavelength range	Flux	Focused beam size	Resolution	Technical Quality Metric
IVU21	4.65 - 25 KeV	0.5 – 2.7 Å	≈ 10^13 p/s @7KeV (hi-flux) ≈ 10^11-10^12 p/s @7KeV (hi-res)	30-70 nm (hi-res) 0.5 µm (hi-flux)	~ 10^{-4}	1

Names of Beamline Personnel and Fractional* FTEs in FY2016

SRX Operations		
YUCHEN	CHENWIEGART	1.03
GARTH	WILLIAMS	1.01
JUERGEN	THIEME	1.00
JAMES	BIANCAROSA	0.37
MIKE	MAKLARY	0.35
	LUCAS	0.21
QINGFU	TANG	0.11
MARY	CARLUCCIDAYTON	0.09
	GAMBELLA	0.08
WAYNE	LEWIS	0.07
SUSAN	MALDONADO	0.07
ROBERT	TODD	0.05
	THEMANN	0.05
42 other staff members contributed effort		0.78
Total		5.26

*Note: 1.0 FTE based on 1760 hours of work. Some staff may log more hours annually

Funding source and fraction of funding for each source FY15-16

FY 2015: DOE – BES; 100%
FY 2016: DOE – BES; 100%
FY 2017: DOE – BES; 100%

Operating funds FY15-16 (K$)

Fiscal Year	Labor Costs	Contract Milestone Payments	Travel	Contract Labor, JT Appts & Shops	Maint/Svc Contracts	Materials & Purchasing	Total Cost
2015	1,679K	19K	39K	47K	10K	110K	1,904K
2016	1,305K	177K	35K	7K	12K	27K	1,562K

Allocation Percentages

Fiscal Year**	Maintenance & Start up	General Users	Partner Users	Facility Staff
2015	79.2	20.1	0	0
2016	46.8	50.5	0	2.7
2017	36	59	0	5

** Partial year for 2017.

Number of unique beamline users each year

Fiscal Year**	General Users	Partner Users	Facility Staff	Total
2015	14	0	6	20
2016	105	0	7	112
2017	64	0	7	71

** Partial year for 2017.

Publications: (all publications used NSLS-II photons; numbers in parentheses indicates staff co-authorship)

Calendar Year**	Refereed	DOE High Profile	DOE High Impact	All Publications
2015	0 (0)	0 (0)	0 (0)	0 (0)
2016	2 (2)	0 (0)	1 (1)	4 (2)
2017	1 (0)	0 (0)	0 (0)	1 (0)

** Partial year for 2017.

Complete List of Publications for CY15-17

(includes publications that used NSLS-II photons, beamline R&D publications by staff, and staff research publications; red text indicates publications that used NSLS-II photons)

Refereed Journal Publications

- G Yadav, J Gallaway, D Turney, M Nyce, J Huang, X Wei, S Banerjee, Regenerable Cu-intercalated MnO2 Layered Cathode for Highly Cyclable Energy Dense Batteries, Nat. Commun., 8, 14424 (2017).
- H Jiang, K Chou, S Petrash, G Williams, J Thieme, D Nykypanchuk, L Li, A Muto, Y Chen-Wiegart, Environmentally Induced Chemical and Morphological Heterogeneity of Zinc Oxide Thin Films, Appl. Phys. Lett.(109), 091909 (2016).
- M Elbakhshwan, S Gill, A Motta, R Weidner, T Anderson, L Ecker, Sample Environment for in situ Synchrotron Corrosion Studies of Materials in Extreme Environments, Rev. Sci. Instrum., 87(10), 105122 (2016).
- J Szlachetko, J Hoszowska, J Dousse, M Nachtegaal, W Blachucki, Y Kayser, J Sa, M Messerschmidt, G Williams, et al., Establishing Nonlinearity Thresholds with Ultraintense X-ray Pulses, Sci. Rep., 6, 33292 (2016).
- B Abbey, R Dilanian, C Darmanin, R Ryan, C Putkunz, A Martin, D Wood, V Streltsov, G Williams, X-Ray Laser–induced Electron Dynamics Observed by Femtosecond Diffraction from Nanocrystals of Buckminsterfullerene, *Science Advances*, 2(9), e1601186 (2016).
- E Stach, Y Li, S Zhao, A Gamalski, D Zakharov, R Tappero, K Chen-Wiegart, J Thieme, U Jung, et al., Characterizing Working Catalysts with Correlated Electron and Photon Probes, Microsc. Microanal., 21, 563-564 (2015).
- A Aquila, A Barty, C Bostedt, S Boutet, G Carini, D dePonte, P Drell, S Doniach, G Williams, et al., The Linac Coherent Light Source Single Particle Imaging Road Map, *ACA Structural Dynamics*, 2(4), 041701 (2015).

Refereed Conference Proceedings

- Y Chen-Wiegart, G Williams, C Zhao, H Jiang, L Li, H Kato, S Petrash, S Centeno, J Thieme, Etc, Early Science Commissioning Results of the Sub-micron Resolution X-ray Spectroscopy Beamline (SRX) in the Field of Materials Science and Engineering, ICXOM23: International Conference on X-ray Optics and Microanalysis, Vol 1764, p. 030004, sponsored by Brookhaven National Laboratory (2016).

Other Publications (books, theses, etc)

- R Palomino, E Stavitski, I Waluyo, Y Chen-Wiegart, M Abeykoon, J Sadowski, J Rodriguez, A Frenkel, S Senanayake, New In-Situ and Operando Facilities for Catalysis Science at NSLS-II: The Deployment of Real-Time, Chemical, and Structure-Sensitive X-ray Probes, Synch. Rad. News, 30(2), 30-37 (2017).

- C Zhao, Synchrotron X-ray Nano-tomography and Fluorescence Microscopy Analysis of Lithium Batteries and Nanoporous Materials for Energy Applications, MS Thesis. Stony Brook University, Stony Brook (2016).
- H Jiang, Evolution of Surface Morphology and Chemistry in ZnO Thin Films and Steel Surfaces studied by Synchrotron X-ray Spectroscopy and Imaging, MS Thesis. Stony Brook University, Stony Brook (2016).

6-BM Materials Measurement (BMM)

Beamline Status

Construction

Overall Description

Scientific Scope

The mission of BMM is to apply X-ray Absorption Spectroscopy (XAS) and X-ray Diffraction (XRD) to the materials science of important societal challenges in energy, health, environment, and national security; to establish structure/function relationships in advanced materials, often at the nanoscale; to accelerate the development of new materials into devices and systems with advanced functionality; and to promote innovation which enhances US industrial competitiveness.

Description

BMM uses a three-pole wiggler source along with a paraboloid collimating mirror, a Si (311) monochromator, and a toroidal focusing mirror to provide light to a highly usable end-station. The end-station is equipped to provide high-quality, high-throughput XAS coordinated with an eight-circle goniometer for XRD and constant-q spectroscopy measurements such as refflexafs or DAFS.

BMM is a partner beamline. The beamline is being constructed and will be operated in partnership with NIST.

Optical System

N/A

Experimental Apparatus

N/A

Computer System

N/A

Current Capabilities Available for Users (as of 1 May 2017)

N/A

Beamline Specifications

Source Type	Energy Range	Wavelength range	Flux	Focused beam size	Resolution	Technical Quality Metric
3PW	4.9-30 KeV		≈ 10^{11} p/s	100 x 100 µm2	~ 10^{-4}	1

Names of Beamline Personnel and Fractional* FTEs in FY2016

*Note: 1.0 FTE based on 1760 hours of work. Some staff may log more hours annually

Funding source and fraction of funding for each source FY15-16

FY 2015: DOC – National Institute of Standards & Technology; 100%
FY 2016: DOC – National Institute of Standards & Technology; 100%
FY 2017: DOC – National Institute of Standards & Technology; 100%

Operating funds FY15-16 (K$)

Fiscal Year	Labor Costs	Contract Milestone Payments	Travel	Contract Labor, JT Appts & Shops	Maint/Svc Contracts	Materials & Purchasing	Total Cost
2015	n/a	n/a	n/a	n/a	n/a	n/a	n/a
2016	n/a	n/a	n/a	n/a	n/a	n/a	n/a

Allocation Percentages

Fiscal Year**	Maintenance & Start up	General Users	Partner Users	Facility Staff
2015	n/a	n/a	n/a	n/a
2016	n/a	n/a	n/a	n/a
2017	n/a	n/a	n/a	n/a

** Partial year for 2017.

Number of unique beamline users each year

Fiscal Year**	General Users	Partner Users	Facility Staff	Total
2015	n/a	n/a	n/a	n/a
2016	n/a	n/a	n/a	n/a
2017	n/a	n/a	n/a	n/a

** Partial year for 2017.

Publications: (all publications used NSLS-II photons; numbers in parentheses indicates staff co-authorship)

Calendar Year**	Refereed	DOE High Profile	DOE High Impact	All Publications
2015	n/a	n/a	n/a	n/a
2016	n/a	n/a	n/a	n/a
2017	n/a	n/a	n/a	n/a

** Partial year for 2017.

Complete List of Publications for CY15-17

(includes publications that used NSLS-II photons, beamline R&D publications by staff, and staff research publications; red text indicates publications that used NSLS-II photons)

Refereed Journal Publications

Refereed Conference Proceedings

Other Publications (books, theses, etc)

7-BM Quick X-ray Absorption and Scattering (QAS)

Beamline Status

Construction

Overall Description

Scientific Scope

QAS will enable the real time study of chemical and physical transformations with sub-second resolution using a combination of x-ray and optical spectroscopy and scattering techniques. It will allow measurement of structure, kinetics and reactivity for the more efficient design of high-activity, high-selectivity, and low-cost catalysts, development of renewable energy conversion technologies, storage of energy products, and portable devices for energy delivery.

Description

QAS will enable the in situ study of chemical and physical transformations using both quick and conventional x-ray absorption and scattering methods. It will allow measurements using separate and combined XAS and XRD techniques, as well as combining these techniques with those provided by end stations with IR and Raman spectroscopy capabilities, in a variety of sample environments

Optical System

A vertical collimating mirror (700mm long) can be switched between two stripes, Rh or Pt. The monochromator can be run in conventional or quick-scan mode and has a Si(111) channel-cut crystal. A toroidal mirror (1000mm long) with Rh coating is used to focus the beam at the sample position.

Experimental Apparatus

Detectors include a PerkinElmer 1621 area detector, a Vortex-ME4 4-element Si-drift, a Canberra multi-element Ge, ion chambersand Canberra PIPS. Sample environments include closed-cycle He refrigerators (T > 10K), in-situ Clausen cells (25°C - 700°C), in-situ Nashner-Adler reaction cells (-150°C - 500°C), a large clam shell furnace reactor (25°C - 900°C), an in-situ high P, high T XAS flow cell (T to 600°C and P to 1200 psi (83 bar)) and an in-situ, custom made XAS-DRIFTS cell (25°C - 700°C). End stations add capabilities for doing DRIFTS/XAS and Raman/XAS.

Computer System

Beamline and endstation motions are controlled by EPICS through Linux IOCs. Linux and Windows workstations are used for detector and sample environment control.

Current Capabilities Available for Users (as of 1 May 2017)

N/A

Beamline Specifications

Source Type	Energy Range	Wavelength range	Flux	Focused beam size	Resolution	Technical Quality Metric
3pw	4.7-31 KeV		$\approx 10^{11}$ - 10^{12} p/s	< 500(V) x 1000(H) µm2	~ 10^{-4}	

Names of Beamline Personnel and Fractional* FTEs in FY2016

*Note: 1.0 FTE based on 1760 hours of work. Some staff may log more hours annually

Funding source and fraction of funding for each source FY15-16

FY 2015: DOE – BES; 100%
FY 2016: DOE – BES; 100%
FY 2017: DOE – BES; 100%

Operating funds FY15-16 (K$)

Fiscal Year	Labor Costs	Contract Milestone Payments	Travel	Contract Labor, JT Appts & Shops	Maint/Svc Contracts	Materials & Purchasing	Total Cost
2015	n/a	n/a	n/a	n/a	n/a	n/a	n/a
2016	n/a	n/a	n/a	n/a	n/a	n/a	n/a

Allocation Percentages

Fiscal Year**	Maintenance & Start up	General Users	Partner Users	Facility Staff
2015	n/a	n/a	n/a	n/a
2016	n/a	n/a	n/a	n/a
2017	n/a	n/a	n/a	n/a

** Partial year for 2017.

Number of unique beamline users each year

Fiscal Year**	General Users	Partner Users	Facility Staff	Total
2015	n/a	n/a	n/a	n/a
2016	n/a	n/a	n/a	n/a
2017	n/a	n/a	n/a	n/a

** Partial year for 2017.

Publications: (all publications used NSLS-II photons; numbers in parentheses indicates staff co-authorship)

Calendar Year**	Refereed	DOE High Profile	DOE High Impact	All Publications
2015	n/a	n/a	n/a	n/a
2016	n/a	n/a	n/a	n/a
2017	n/a	n/a	n/a	n/a

** Partial year for 2017.

Complete List of Publications for CY15-17

(includes publications that used NSLS-II photons, beamline R&D publications by staff, and staff research publications; red text indicates publications that used NSLS-II photons)

Refereed Journal Publications

Refereed Conference Proceedings

Other Publications (books, theses, etc)

7-ID-1 Spectroscopy Soft and Tender (SST-1)

Beamline Status

Construction

Overall Description

Scientific Scope

The mission of SST is to apply X-ray Photoelectron Spectroscopy (XPS) and Near Edge X-ray Absorption Fine Structure (NEXAFS) spectroscopy to the materials science of important societal challenges in energy, health, environment, and national security; to establish structure/function relationships in advanced materials, often at the nanoscale; to accelerate the development of new materials into devices and systems with advanced functionality; and to promote innovation which enhances US industrial competitiveness.

Description

SST will have 6 unique world class NEXAFS/XPS experimental stations: 2 full field microscopes, 2 automated high-throughput stations, and 2 in-situ high pressure stations. Soft and tender beams will enable a continuous selection of X-rays from 100 eV to 7.5 keV at a common focal point in a single experiment (unique capability, enhancing depth selectivity in XPS or HAXPES).

SST is a partner beamline. This beamline is being constructed and operated in partnership with NIST.

Optical System

N/A

Experimental Apparatus

N/A

Computer System

N/A

Current Capabilities Available for Users (as of 1 May 2017)

N/A

Beamline Specifications

Source Type	Energy Range	Wavelength range	Flux	Focused beam size	Resolution	Technical Quality Metric
EPU60	100-2200 eV		10^{12}-10^{13} photons/s	variable down to 10 µm	~ 10^{-4}	1

Names of Beamline Personnel and Fractional* FTEs in FY2016

*Note: 1.0 FTE based on 1760 hours of work. Some staff may log more hours annually

Funding source and fraction of funding for each source FY15-16

FY 2015: DOC – National Institute of Standards & Technology; 100%
FY 2016: DOC – National Institute of Standards & Technology; 100%
FY 2017: DOC – National Institute of Standards & Technology; 100%

Operating funds FY15-16 (K$)

Fiscal Year	Labor Costs	Contract Milestone Payments	Travel	Contract Labor, JT Appts & Shops	Maint/Svc Contracts	Materials & Purchasing	Total Cost
2015	n/a	n/a	n/a	n/a	n/a	n/a	n/a
2016	n/a	n/a	n/a	n/a	n/a	n/a	n/a

Allocation Percentages

Fiscal Year**	Maintenance & Start up	General Users	Partner Users	Facility Staff
2015	n/a	n/a	n/a	n/a
2016	n/a	n/a	n/a	n/a
2017	n/a	n/a	n/a	n/a

** Partial year for 2017.

Number of unique beamline users each year

Fiscal Year**	General Users	Partner Users	Facility Staff	Total
2015	n/a	n/a	n/a	n/a
2016	n/a	n/a	n/a	n/a
2017	n/a	n/a	n/a	n/a

** Partial year for 2017.

Publications: (all publications used NSLS-II photons; numbers in parentheses indicates staff co-authorship)

Calendar Year**	Refereed	DOE High Profile	DOE High Impact	All Publications
2015	n/a	n/a	n/a	n/a
2016	n/a	n/a	n/a	n/a
2017	n/a	n/a	n/a	n/a

** Partial year for 2017.

Complete List of Publications for CY15-17

(includes publications that used NSLS-II photons, beamline R&D publications by staff, and staff research publications; red text indicates publications that used NSLS-II photons)

Refereed Journal Publications

Refereed Conference Proceedings

Other Publications (books, theses, etc)

7-ID-2 Spectroscopy Soft and Tender (SST-2)

Beamline Status

Construction

Overall Description

Scientific Scope

The mission of SST is to apply X-ray Photoelectron Spectroscopy (XPS) and Near Edge X-ray Absorption Fine Structure (NEXAFS) spectroscopy to the materials science of important societal challenges in energy, health, environment, and national security; to establish structure/function relationships in advanced materials, often at the nanoscale; to accelerate the development of new materials into devices and systems with advanced functionality; and to promote innovation which enhances US industrial competitiveness.

Description

SST will have 6 unique world class NEXAFS/XPS experimental stations: 2 full field microscopes, 2 automated high-throughput stations, and 2 in-situ high pressure stations. Soft and tender beams will enable a continuous selection of X-rays from 100 eV to 7.5 keV at a common focal point in a single experiment (unique capability, enhancing depth selectivity in XPS or HAXPES).

SST-2 is a partner beamline. Beamline construction and operation are done in partnership with NIST.

Optical System

N/A

Experimental Apparatus

N/A

Computer System

N/A

Current Capabilities Available for Users (as of 1 May 2017)

N/A

Beamline Specifications

Source Type	Energy Range	Wavelength range	Flux	Focused beam size	Resolution	Technical Quality Metric
U42	1-7.5 KeV		10^{12}-10^{13} photons/s	variable down to 10 µm	~ 10^{-4}	1

Names of Beamline Personnel and Fractional* FTEs in FY2016

*Note: 1.0 FTE based on 1760 hours of work. Some staff may log more hours annually

Funding source and fraction of funding for each source FY15-16

FY 2015: DOC – National Institute of Standards & Technology; 100%
FY 2016: DOC – National Institute of Standards & Technology; 100%
FY 2017: DOC – National Institute of Standards & Technology; 100%

Operating funds FY15-16 (K$)

Fiscal Year	Labor Costs	Contract Milestone Payments	Travel	Contract Labor, JT Appts & Shops	Maint/Svc Contracts	Materials & Purchasing	Total Cost
2015	n/a	n/a	n/a	n/a	n/a	n/a	n/a
2016	n/a	n/a	n/a	n/a	n/a	n/a	n/a

Allocation Percentages

Fiscal Year**	Maintenance & Start up	General Users	Partner Users	Facility Staff
2015	n/a	n/a	n/a	n/a
2016	n/a	n/a	n/a	n/a
2017	n/a	n/a	n/a	n/a

** Partial year for 2017.

Number of unique beamline users each year

Fiscal Year**	General Users	Partner Users	Facility Staff	Total
2015	n/a	n/a	n/a	n/a
2016	n/a	n/a	n/a	n/a
2017	n/a	n/a	n/a	n/a

** Partial year for 2017.

Publications: (all publications used NSLS-II photons; numbers in parentheses indicates staff co-authorship)

Calendar Year**	Refereed	DOE High Profile	DOE High Impact	All Publications
2015	n/a	n/a	n/a	n/a
2016	n/a	n/a	n/a	n/a
2017	n/a	n/a	n/a	n/a

** Partial year for 2017.

Complete List of Publications for CY15-17

(includes publications that used NSLS-II photons, beamline R&D publications by staff, and staff research publications; red text indicates publications that used NSLS-II photons)

Refereed Journal Publications

Refereed Conference Proceedings

Other Publications (books, theses, etc)

8-BM Tender Energy X-ray Absorption Spectroscopy (TES)

Beamline Status

Commissioning

Overall Description

Scientific Scope

Applications of spatially resolved and in-situ XAFS and imaging in the 1-5 keV energy range, in a variety of fields particularly energy and climate sciences.

Beamline Description

TES is a tender-energy beamline optimized for spatially resolved and in-situ XAFS and imaging in the 1-5 keV energy range, in a non-vacuum sample environment.

Optical System

A pair of mirrors with adjustable pitch for vertical collimation and harmonic rejection; a double-crystal monochromator; a toroidal focusing mirror for sub-mm spot size; a custom KB mirror system for microbeam.

Experimental Apparatus

Helium sample environment with Ge and Vortex fluorescence detectors, I-zero and transmission ion chambers, feedthroughs for in-situ electrochemistry; catalysis sample environment under development.

Computer System

User interface for collection of on-the-fly images and step or on-the-fly energy scanning for standard or quick XAS.

Current Capabilities Available for Users (as of 1 May 2017)

- X-ray Fluorescence Microprobe XANES and elemental imaging, in ROI/Scaler mode, with a beam size user-tunable from 3x3 to 15x60 microns, 2-5 keV energy range, helium sample environment, room temperature.
- Extending energy range lower (to 1.7-2.5 keV for Si K-edge), or higher (up to 8 keV) for X-ray Fluorescence Microprobe
- Microbeam EXAFS (extended energy scanning)
- Development of in-situ or special sample cells for X-ray Fluorescence microprobe at 2-5 keV, overall He environment

Beamline Specifications

Source Type	Energy Range	Wavelength range	Flux	Focused beam size	Resolution	Technical Quality Metric
Dipole	1-8 KeV		up to $2x10^{12}$ p/s macro, up to 10^{12} p/s micro	1 -100 µm micro, 100 - 1000 µm macro	~ 10^{-4}	

Names of Beamline Personnel and Fractional* FTEs in FY2016

TES Operations		
PAUL	NORTHRUP	0.07
SUSAN	MALDONADO	0.07
2 other staff members contributed effort		0.03
Total		0.17

*Note: 1.0 FTE based on 1760 hours of work. Some staff may log more hours annually

Funding source and fraction of funding for each source FY15-16

FY 2015: DOE – BES; 100%
FY 2016: DOE – BES; 100%
FY 2017: DOE – BES; 100%

Operating funds FY15-16 (K$)

Fiscal Year	Labor Costs	Contract Milestone Payments	Travel	Contract Labor, JT Appts & Shops	Maint/Svc Contracts	Materials & Purchasing	Total Cost
2015	n/a	n/a	n/a	n/a	n/a	n/a	n/a
2016	35K		2K				38K

Allocation Percentages

Fiscal Year**	Maintenance & Start up	General Users	Partner Users	Facility Staff
2015	n/a	n/a	n/a	n/a
2016	n/a	n/a	n/a	n/a
2017	81	17	0	2

** Partial year for 2017.

Number of unique beamline users each year

Fiscal Year**	General Users	Partner Users	Facility Staff	Total
2015	n/a	n/a	n/a	n/a
2016	1	0	2	3
2017	18	0	4	22

** Partial year for 2017.

Publications: (all publications used NSLS-II photons; numbers in parentheses indicates staff co-authorship)

Calendar Year**	Refereed	DOE High Profile	DOE High Impact	All Publications
2015	n/a	n/a	n/a	n/a
2016	0 (0)	0 (0)	0 (0)	0 (0)
2017	0 (0)	0 (0)	0 (0)	1 (0)

** Partial year for 2017.

Complete List of Publications for CY15-17

(includes publications that used NSLS-II photons, beamline R&D publications by staff, and staff research publications; red text indicates publications that used NSLS-II photons)

Refereed Journal Publications

- P Northrup, A Leri, R Tappero, Applications of "Tender" Energy (1-5 keV) X-ray Absorption Spectroscopy in Life Sciences, Protein Peptide Lett., 23(3), 300-308 (2016).
- J Moon, P Kalb, L Milian, P Northrup, Characterization of a Sustainable Sulfur Polymer Concrete Using Activated Fillers, 67, 20-29 (2016).
- A Leri, L Mayer, K Thornton, P Northrup, M Dunigan, K Ness, A Gellis, A Marine Sink for Chlorine in Natural Organic Matter, Nature Geosci., 8, 620-624 (2015).
- D Abdala, P Northrup, Y Arai, D Sparks, Surface Loading Effects on Orthophosphate Surface Complexation at the Goethite/water Interface as Examined by Extended X-ray Absorption Fine Structure (EXAFS) Spectroscopy, J. Colloid Interface Sci., 437, 297-303 (2015). [107456]

- D Abadala, P Northrup, E Cesar Vicentin, D Sparks, Residence Time and pH Effects on the Bonding Configuration of Orthophosphate Surface Complexes at the Goethite/water Interface as Examined by Extended X-ray Absorption Fine Structure (EXAFS) Spectroscopy, J. Colloid Interface Sci., 442, 15-21 (2015).
- Yu, H Pan, Y Zhou, P Northrup, J Xiao, S Bak, M Liu, K Nam, X Yang, et al., Direct Observation of the Redistribution of Sulfur and Polysufides in Li-S Batteries During First Cycle by In Situ X-ray Fluorescence Microscopy, Adv. Energy Mater., 5(16), 1500072 (2015).

Other Publications (books, theses, etc)

- A Gamble, Speciation and Reactivity of Phosphorus and Arsenic in Mid-Atlantic Soils, Ph.D. Thesis. University of Delaware, Newark (2017).

8-ID Inner-Shell Spectroscopy (ISS)

Beamline Status

Operations

Overall Description

Scientific Scope

The beamline provides in-situ and operando experimental tools which are optimized for fast X-ray spectroscopy including XAFS and inelastic techniques.

Beamline Description

The ISS beamline, a high flux damping wiggler spectroscopy beamline, is part of the NEXT project and available in FY 2017 for general user operations. To make state-of-the-art spectroscopic tools available and combine the necessary instrumentation with in-situ and operando instrumentation for energy research, materials sciences, and biological research is goal of the ISS beamline.

Optical System

The optical system is using a filter box, collimation mirror system, a high heat load double crystal monochromator, an optional high resolution channel cut monochromator, an optional focusing mirror, a higher harmonics rejection mirror system, and a poly-capillary focusing unit.

Experimental Apparatus

The user have the choice between a highly engineered sample and detection unit optimized for in-situ and operando experiments and an "empty" hutch which allows to implement complex and large sample environments.

Computer System

Centralized data storage and analysis system providing Linux and Windows support.

Current Capabilities Available for Users (as of 1 May 2017)

- EXAFS in transmission and total fluorescence mode
- operando experiments in the field of fuel-cell and battery research
- heterogeneous catalysis with diluted gases (up to 2 bar gas pressure and with non-flammable, non-toxic, and non-explosion dilution limit)
- partial fluorescence XAS
- heterogeneous catalysis with concentrated gases
- high throughput experiments (ex-situ EXAFS in transmission and total fluorescence mode)
- modulation spectroscopy

Beamline Specifications

Source Type	Energy Range	Wavelength range	Flux	Focused beam size	Resolution	Technical Quality Metric
DW100	4.9 - 36 KeV		≈ 10^{14} p/s	25 x 25 µm2	10^{-5} - 10^{-4}	1

Names of Beamline Personnel and Fractional* FTEs in FY2016

ISS Operations		
BRUNO	VALDRIGHILUVIZOTTO	0.41
ILYA	STAVITSKI	0.14
KLAUS	ATTENKOFER	0.11
HARMANPREET	BASSAN	0.09
SUSAN	MALDONADO	0.07
15 other staff members contributed effort		0.08
Total		0.89

*Note: 1.0 FTE based on 1760 hours of work. Some staff may log more hours annually

Funding source and fraction of funding for each source FY15-16

FY 2015: DOE – BES; 100%
FY 2016: DOE – BES; 100%
FY 2017: DOE – BES; 100%

Operating funds FY15-16 (K$)

Fiscal Year	Labor Costs	Contract Milestone Payments	Travel	Contract Labor, JT Appts & Shops	Maint/Svc Contracts	Materials & Purchasing	Total Cost
2015	n/a	n/a	n/a	n/a	n/a	n/a	n/a
2016	203K		11K	1 k		10K	224K

Allocation Percentages

Fiscal Year**	Maintenance & Start up	General Users	Partner Users	Facility Staff
2015	n/a	n/a	n/a	n/a
2016	91	9	0	0
2017	54	46	0	0

** Partial year for 2017.

Number of unique beamline users each year

Fiscal Year**	General Users	Partner Users	Facility Staff	Total
2015	n/a	n/a	n/a	n/a
2016	11	0	4	15
2017	49	0	3	52

** Partial year for 2017.

Publications: (all publications used NSLS-II photons; numbers in parentheses indicates staff co-authorship)

Calendar Year**	Refereed	DOE High Profile	DOE High Impact	All Publications
2015	n/a	n/a	n/a	n/a
2016	1 (0)	0 (0)	1 (0)	1 (0)
2017	0 (0)	0 (0)	0 (0)	0 (0)

** Partial year for 2017.

Complete List of Publications for CY15-17

(includes publications that used NSLS-II photons, beamline R&D publications by staff, and staff research publications; red text indicates publications that used NSLS-II photons)

Refereed Journal Publications

- R Palomino, E Stavitski, I Waluyo, Y Chen-Wiegart, M Abeykoon, J Sadowski, J Rodriguez, A Frenkel, S Senanayake, New In-Situ and Operando Facilities for Catalysis Science at NSLS-II: The Deployment of Real-Time, Chemical, and Structure-Sensitive X-ray Probes, Synch. Rad. News, 30(2), 30-37 (2017).
- J Li, A Alsudairi, Z Ma, S Mukerjee, Q Jia, Asymmetric Volcano Trend in Oxygen Reduction Activity of Pt and Non-Pt Catalysts: In Situ Identification of the Site-Blocking Effect, J. Am. Chem. Soc., 139(4), 1384–1387 (2016).
- A Colli, K Attenkofer, B Raghothamachar, M Dudley, Synchrotron X-Ray Topography for Encapsulation Stress/Strain and Crack Detection in Crystalline Silicon Modules, IEEE J. Photovoltaics, 6(5), 1387-1389 (2016).

- J Rogers, M Mangarella, A D'Amico, J Gallagher, M Dutzer, E Stavitski, J Miller, C Sievers, Differences in the Nature of Active Sites for Methane Dry Reforming and Methane Steam Reforming over Nickel Aluminate Catalysts, ACS Catal., 6, 5873-5886 (2016).
- M Popecki, d Bennis, B Adams, A O'Mahony, C Craven, M Foley, M Minot, J Renaud, K Attenkofer, et al., Development of Polycapillary X-ray Optics for Synchrotron spectroscopy, Advances in X-Ray/EUV Optics and Components X, Vol 9588, sponsored by Shunji Goto; Christian Morawe; Ali M. Khounsary (2015).
- M Popecki, D Bennis, B Adams, A O'Mahony, C Craven, M Foley, M Minot, J Renaud, K Attenkofer, et al., Development of Polycapillary X-ray Optics for Synchrotron Spectroscopy, Advances in X-Ray/EUV Optics and Components X, 95880D , Vol 9588, sponsored by Shunji Goto; Christian Morawe; Ali M. Khounsary (2015).
- S Canton, X Zhang, Y Liu, J Zhang, M Papai, A Corani, A Smeigh, G Smolentsev, K Attenkofer, et al., Watching the Dynamics of Electrons and Atoms at Work in Solar Energy Conversion, Faraday Discuss, 185, 51-68 (2015).
- P Serra-Crespo, A Dikhtiarenko, E Stavitski, J Juan-Alcañiz, F Kapeteijn, F Coudert, K Gason, Experimental Evidence of Negative Linear Compressibility in the MIL-53 Metal–Organic Framework Family, CrystEngComm, 17(2), 185-472 (2015). [107485]
- P Serra-Crespo, A ikhtiarenko, E Stavitski, J Juan-Alcañiz, F Kapteijn, F Coudert, J Gascon, Experimental Evidence of Negative Linear Compressibility in the MIL-53 Metal–organic Framework Family, CrystEngComm, 17(2), 276-280 (2015). [107485]
- P Gelfand, R Smith, E Stavitski, D Borchelt, L Miller, Characterization of Protein Structural Changes in Living Cells Using Time-Lapsed FTIR Imaging, Anal. Chem., 87(12), 6025-6021 (2015).
- S Zhao, Y Li, E Stavitski, R Tappero, S Crowley, M J Castaldi, D N Zakharov, R G Nuzzo, A I Frenkel, E A Stach, Operando Characterization of Catalysts with a Portable Microreactor, ChemCatChem, 7(22), 3683-3691 (2015). [108512]
- P Warnicke, E Stavitski, J Lee, A Yang, Z Chen, X Zou, S Zohar, W Bailey, V Harris, D Arena, Direct Observation of Symmetry-specific Precession in a Rerrimagnet, Phys. Rev. B: Condens. Matter, 92, 104402 (2015).

Other Publications (books, theses, etc)

- R Palomino, E Stavitski, I Waluyo, Y Chen-Wiegart, M Abeykoon, J Sadowski, J Rodriguez, A Frenkel, S Senanayake, New In-Situ and Operando Facilities for Catalysis Science at NSLS-II: The Deployment of Real-Time, Chemical, and Structure-Sensitive X-ray Probes, Synch. Rad. News, 30(2), 30-37 (2017).

10-ID Inelastic X-ray Scattering (IXS)

Beamline Status

Operations

Overall Description

Scientific Scope

IXS is dedicated to inelastic x-ray scattering studies of vibrational dynamics in a broad range of material systems at nm length scale and picosecond to sub-picosecond time with ~meV energy resolution, sharp spectral contrast and excellent momentum resolution (0.1 nm^{-1}) at a moderate energy of 9.1 keV that capitalizes on NSLS-II's strengths in flux and brightness. The key instrument is a novel spectrometer with analyzer optics based on the combination of a collimating Montel mirror and highly dispersive back-reflection flat crystal optics on a spectrometer arm that covers a wide range of momentum transfers, providing unique research strengths in soft matters and bio-molecular systems with mesoscopic complexity and inhomogeneity, as well as powerful performance for the study of relaxation dynamics, sound propagation and transport properties, and phonons in single crystals, surfaces, thin films, confined liquids, and systems in extreme pressure and temperature.

Beamline Description

IXS utilizes a room-temperature 3-m long in-vacuum undulator source with a magnet period of 22 mm, installed at 10-ID, a high-β long straight section. The device delivers a peak spectral flux of ~8 $x10^{14}$ photons/sec/0.1%bw at 9.13 keV at 500 mA operation current

Optical System

The beamline optical system includes a compound refractive lens to pre-focus and a double crystal high heat load monochromator to pre-monochromatize the beam before it is delivered to the high-resolution monochromator based on a four bounces scheme. The monochromatic beam is focused by a set of KB mirrors to the sample. The analyzer optical system, mounted on the spectrometer arm, includes a Montel multilayer collimating mirror collecting the photons scattered by the sample with a large angular acceptance and delivering them to the CDW analyzer based on asymmetric dispersive crystal optics. The analyzed x-ray photons are recorded by a 2D strip detector.

Experimental Apparatus

Novel IXS spectrometer with collimating Montel mirror and highly-dispersive back-reflection analyzer crystal optics for ~meV resolution. High-pressure low-temperature cryostat with online Ruby system for in-situ experiments. Humidity and temperature controlled sample chamber for

biological materials. Imaging detector for on-line sample alignment and phase characterization by x-ray diffraction.

Computer System

Beamline components are controlled by EPICS. The user interface is implemented using Python and Control System Studio (CSS) clients operating under Linux Debian workstations.

Current Capabilities Available for Users (as of 1 May 2017)

Inelastic X-ray scattering with an energy resolution of 1.5 – 2.0 meV with Gaussian-like tails and a momentum resolution of up to 0.2 nm-1. Available sample environments include low temperature cryostat to 5 K and humidity (up to 97.5%) and temperature (20 – 50 deg C) control chamber for biological materials.

Eulerian cradle and low-temperature sample environment down to 2 K.

Beamline Specifications

Source Type	Energy Range	Wavelength range	Flux	Focused beam size	Resolution	Technical Quality Metric
IVU22	9.13 KeV		~ 10^{10} p/s	5 x 7 µm2	~1 meV	1

Names of Beamline Personnel and Fractional* FTEs in FY2016

IXS Operations		
ALESSANDRO	CUNSOLO	1.06
ALEXEY	SUVOROV	1.05
YONG	CAI	1.03
DAVID	COBURN	0.37
KAZIMIERZ	GOFRON	0.29
DAVID	LEVY	0.25
STEPHEN	ANTONELLI	0.22
RICHARD	GREENE	0.21
JOSEPH	SULLIVAN	0.12
ANDREW	DESANTIS	0.11
MARY	CARLUCCIDAYTON	0.09
SUSAN	MALDONADO	0.07
LEO	REFFI	0.06
DENNIS	POSHKA	0.05
45 other staff members contributed effort		0.91
Total		5.87

*Note: 1.0 FTE based on 1760 hours of work. Some staff may log more hours annually

Funding source and fraction of funding for each source FY15-16

FY 2015: DOE – BES; 100%
FY 2016: DOE – BES; 100%
FY 2017: DOE – BES; 100%

Operating funds FY15-16 (K$)

Fiscal Year	Labor Costs	Contract Milestone Payments	Travel	Contract Labor, JT Appts & Shops	Maint/Svc Contracts	Materials & Purchasing	Total Cost
2015	1,971K	55K	23K	115K	72K	151K	2,387K
2016	1,586K	0	28K	18K	25K	127K	1,784K

Allocation Percentages

Fiscal Year**	Maintenance & Start up	General Users	Partner Users	Facility Staff
2015	100	0	0	0
2016	56.4	40.2	0	3.4
2017	33	60	0	7

** Partial year for 2017.

Number of unique beamline users each year

Fiscal Year**	General Users	Partner Users	Facility Staff	Total
2015	0	0	7	7
2016	15	0	7	22
2017	9	0	6	15

** Partial year for 2017.

Publications: (all publications used NSLS-II photons; numbers in parentheses indicates staff co-authorship)

Calendar Year**	Refereed	DOE High Profile	DOE High Impact	All Publications
2015	0 (0)	0 (0)	0 (0)	0 (0)
2016	0 (0)	0 (0)	0 (0)	0 (0)
2017	0 (0)	0 (0)	0 (0)	0 (0)

** Partial year for 2017.

Complete List of Publications for CY15-17

(includes publications that used NSLS-II photons, beamline R&D publications by staff, and staff research publications; red text indicates publications that used NSLS-II photons)

Refereed Journal Publications

- A Suvorov, A Cunsolo, O Chubar, Y Cai, Ultrahigh Energy Resolution Focusing Monochromator for Inelastic X-Ray Scattering Spectrometer, Opt. Express, 23(24), 31607-31618 (2015).
- M Zhernenkov, D Bolmatov, D Soloviov, K Zhernenkov, B Toperverg, A Cunsolo, A Bosak, Y Cai, Revealing the Mechanism of Passive Transport in Lipid Bilayers via Phonon-mediated Nanometre-scale Density Fluctuations, Nat. Commun., 7, 11575 (2016). [108276]
- D Bolmatov, M Zhernenkov, D Zav'yalov, S Stoupin, A Cunsolo, Y Cai, Thermally Triggered Phononic Gaps in Liquids at THz Scale, Sci. Rep., 6, 19469 (2016). [108070]
- A Cunsolo, A Suvorov, Y Cai, The Onset of Shear Modes in the High Frequency Spectrum of Simple Disordered Systems: Current Knowledge and Perspectives, Philos. Mag. A, 96(7-9), 732-742 (2016).
- D Bolmatov, M Zhernenkov, D Zav'yalov, Y Cai, A Cunsolo, Terasonic Excitations in 2D Gold Nanoparticle Arrays in a Water Matrix as Revealed by Atomistic Simulations, J. Phys. Chem. C, 120(35), 19896–19903 (2016). [112690]
- M Honnicke, L Bianco, S Ceppi, C Cusatis, X Huang, Y Cai, G Stutz, Construction of a Quartz Spherical Analyzer: Application to High-resolution Analysis of the Ni K-alpha Emission Spectrum, J. Appl. Cryst., 49(5), 1443-1453 (2016).
- S Bellissima, S De Panfilis, U Bafile, A Cunsolo, M Gonzalez, E Guarini, F Formisano, The Hydrogen-bond Collective Dynamics in Liquid Methanol, Sci. Rep., 6, 39533 (2016).
- A Cunsolo, The Spectrum of Density Fluctuations of Noble Gases Probed by THz Neutron and X-ray Spectroscopy, 6(3), 64 (2016).
- A Cunsolo, Using X-ray as a Probe of the Terahertz Dynamics of Disordered Systems – Complementarity with Inelastic Neutron Scattering and Future Perspectives, Neutron Scattering, p. 1-36, InTech, Rjeka (2016).
- D Bolmatov, M Zhernenkov, D Zav'yalov, S Tkachev, A Cunsolo, Y Cai, The Frenkel Line: a Direct Experimental Evidence for the New Thermodynamic Boundary, Sci. Rep., 5, 15850 (2015). [107811]
- D Bolmatov, M Zhernenkov, D Zav'yalov, S Stoupin, Y Cai, A Cunsolo, Revealing the Mechanism of the Viscous-to-Elastic Crossover in Liquids, J. Phys. Chem. Letts., 6(15), 3048–3053 (2015). [108218]
- D Bolmatov, D Zav'yalov, M Zhernenkov, E Musaev, Y Cai, Unified Phonon-based Spproach to the Thermodynamics of Solid, Liquid and Gas States, 363, 221-242 (2015).

- K Smith, J Poulsen, J Nyman, A Cunsolo, P Rossky, Application of a New Ensemble Conserving Quantum Dynamics Simulation Algorithm to Liquid Para-hydrogen and Ortho-deuterium, J. Chem. Phys., 142(24), 244113 (2015).
- A Cunsolo, The THz Spectrum of Density Fluctuations of Water: The Viscoelastic Regime, 2015(137435), 1-24 (2015).

Refereed Conference Proceedings

- K Gofron, Y Cai, D Coburn, S Antonelli, J Flores, A Suvorov, On-axis Microscopes for the Inelastic X-ray Scattering Beamline at NSLS-II, J of Phys: Conf Series (12th International Conference on Synchrotron Radiation Instrumentation), Vol 1741, p. 030027, sponsored by NSLS-II (2016).
- A Suvorov, Y Cai, Simulation of an IXS Imaging Analyzer with an Extended Scattering Source, Proceedings of SPIE: Advances in X-ray/EUV Optics and Components XI, Vol 9963, p. 99630A, sponsored by SPIE (2016).

11-BM Complex Materials Scattering (CMS)

Beamline Status

Commissioning

Overall Description

Scientific Scope

CMS aims to facilitate rational design and discovery of new functional materials by unravelling the relations between constituents, processing, structure, and properties. To this end, CMS specializes in x-ray scattering-based nano- and mesoscale characterization of the bulk and interfacial structures of complex, hierarchical materials, including nanomaterials, soft matter, and biomolecular materials. A long-term goal of CMS is to enable materials design and discovery based on intelligent, efficient exploration of materials structure in large parameter spaces.

Beamline Description

CMS provides instrumentation for simultaneous small- and wide-angle x-ray scattering (SAXS, WAXS) as well as scattering in grazing incidence geometry (GISAXS, GIWAXS), giving access to complementary information at multiple length scales ranging from Angstroms to submicrons. In addition, the moderate microfocusing capability enables scanning microbeam characterization of heterogeneous materials at resolutions of tens of microns. The beamline will also develop capabilities for automation-aided intelligent exploration of vast parameter spaces.

Optical System

Double multilayer monochromator. Primary toroidal focusing mirror. Secondary KB mirrors.

Experimental Apparatus

Area detectors: Pilatus 300k for SAXS (to be upgraded to Pilatus 2M in summer 2017); Photonic Sciences in-vacuum CCD for WAXS.
Ion chambers, scintillatior, diamond diode, and photo diodes for beam intensity monitoring.
Computer-controlled sample position, tilt, and rotation stages.
Temperature-controlled sample holders for array of capillaries and thin films.
Option for in-vacuum sample environment.
On-axis and off-axis sample viewing.

Computer System

Beamline components are controlled by EPICS. The user interface is through CSS-Studio and Python clients. The user views the experimental system (sample and the surrounding

environment) through CCD-coupled optical microscopes using Prosilica cameras. Linux Debian running IOCs. Dedicated Linux and Windows computers for area detectors.

Current Capabilities Available for Users (as of 1 May 2017)

- Small-angle X-ray scattering (transmission or grazing-incidence)
- Wide-angle X-ray scattering (transmission or grazing-incidence)
- High-throughput measurements for capillaries (SAXS/WAXS) or thin films (GISAXS/GIWAXS), based on robotic sample handling (room temperature)

Beamline Specifications

Source Type	Energy Range	Wavelength range	Flux	Focused beam size	Resolution	Technical Quality Metric
3PW	10-17 keV	0.7 - 1.2 Å	≈ 10^{10} - 10^{12} p/s	100 x 200 µm2 (no KB); 25 x 50 µm2 (KB)	~ 10^{-2}	

Names of Beamline Personnel and Fractional* FTEs in FY2016

CMS Operations		
MASAFUMI	FUKUTO	0.07
SUSAN	MALDONADO	0.07
5 other staff members contributed effort		0.07
Total		0.21

*Note: 1.0 FTE based on 1760 hours of work. Some staff may log more hours annually

Funding source and fraction of funding for each source FY15-16

FY 2015: DOE – BES; 100%
FY 2016: DOE – BES; 100%
FY 2017: DOE – BES; 100%

Operating funds FY15-16 (K$)

Fiscal Year	Labor Costs	Contract Milestone Payments	Travel	Contract Labor, JT	Maint/Svc	Materials &	Total Cost

				Appts & Shops	Contracts	Purchasing	
2015	n/a	n/a	n/a	n/a	n/a	n/a	n/a
2016	48K					24K	72K

Allocation Percentages

Fiscal Year**	Maintenance & Start up	General Users	Partner Users	Facility Staff
2015	n/a	n/a	n/a	n/a
2016	n/a	n/a	n/a	n/a
2017	65	29	4	2

** Partial year for 2017.

Number of unique beamline users each year

Fiscal Year**	General Users	Partner Users	Facility Staff	Total
2015	n/a	n/a	n/a	n/a
2016	0	1	4	5
2017	47	0	4	51

** Partial year for 2017.

Publications: (all publications used NSLS-II photons; numbers in parentheses indicates staff co-authorship)

Calendar Year**	Refereed	DOE High Profile	DOE High Impact	All Publications
2015	n/a	n/a	n/a	n/a
2016	0 (0)	0 (0)	0 (0)	0 (0)
2017	0 (0)	0 (0)	0 (0)	0 (0)

** Partial year for 2017.

Complete List of Publications for CY15-17

(includes publications that used NSLS-II photons, beamline R&D publications by staff, and staff research publications; red text indicates publications that used NSLS-II photons)

Refereed Journal Publications

- M Fukuto, L Yang, D Nykypanchuk, I Kuzmenko, Transmission X-ray Scattering as a Probe for Complex Liquid-surface Structures, J. Synch. Rad., 23, 519-531 (2016). [108469]

- N Jiang, L Sendogdular, M Sen, M Endoh, T Koga, M Fukuto, B Akgun, S Satija, C Nam, Novel Effects of Compressed CO2 Molecules on Structural Ordering and Charge Transport in Conjugated Poly(3-hexylthiophene) Thin Films, Langmuir, 32(42), 10851-10860 (2016).
- M Fukuto, B Ocko, D Bonthuis, R Netz, H Sternruck, D Pointoni, I Kuzmenko, J Haddad, M Deutsch, Nanoscale Structure of the Oil-Water Interface, Phys. Rev. Lett., 117(25), 256102 (2016).

11-ID Coherent Hard X-ray Scattering (CHX)

Beamline Status

Operations

Overall Description

Scientific Scope

The Coherent Hard X-ray Scattering (CHX) beamline is dedicated to studies of nanometer-scale dynamics in materials using x-ray photon correlation spectroscopy (XPCS) with world-leading hard x-ray coherent flux and a detection system for fast dynamics into the sub-millisecond regime.

XPCS is based on measuring time correlation functions of the speckle fluctuations that occur when a coherent x-ray beam is scattered from a disordered sample. It can be used to measure equilibrium dynamics via the "usual" single- speckle intensity-intensity autocorrelation functions $g^{(2)}(q, t)$. When combined with 2D area detectors and a multispeckle detection technique, it can also be used to measure non-stationary, non-equilibrium dynamics via two-time correlation functions $g^{(2)}(q, t_1, t_2)$. Higher-order correlation functions $g^{(n)(q, t)}$ can be used to characterize heterogeneities in the dynamical properties. The key quantity that enables XPCS experiments is the source brightness. This determines the flux of coherent x-ray photons and ultimately the signal-to-noise ratio (SNR) of the measured correlation functions. With the unprecedented brilliance of the NSLS-II storage ring exceeding 1021 ph/s/mrad2/mm2/0.1% bandwidth at 8 keV, the CHX beamline will allow studies of dynamics on time scales that can be 100 times faster and on shorter length scales than currently achievable elsewhere.

Beamline Description

The CHX beamline is dedicated to studies of the nano-scale and meso-scale dynamics of materials using coherent X-ray scattering. As a result of the unprecedented source brightness, this beamline will enable measurements on time scales that can be several orders of magnitude faster than what is achievable at current facilities.

Optical System

The first optical element is a water-cooled horizontally deflecting flat mirror at fixed incidence angle (HDM). The cryo-cooled, pseudo-channel-cut Double Crystal Monochromator (DCM) provides a choice of Si111 or Si220 crystals in vertical scattering geometry. The crystals can be completely removed from the beam for operation with a wider band-pass monochromatic beam using the Double Multilayer Monochromator (DMM). The DMM houses two sets of substrates in horizontal reflection geometry, one set is coated with multilayers, while the other set provides bare and Rh coated Si stripes for use as a Harmonic Rejection Mirror (HRM) in monochromatic

operation mode. It is also possible to remove both DMM and HRM completely from the beam (this is the most likely 'day 1' operating mode).

Vertical focusing of the X-ray beam in a x:y geometry is accomplished by water-cooled 1D compound refractive lenses. To achieve nearly achromatic focusing, different sets of lenses are available in a so-called Transfocator that also exhibits a large travel range along the beam direction. A safety shutter is located at the end of the FOE that allows keeping the high heat load synchrotron beam on the optical elements while entering the endstation.

The CHX endstation is equipped with two kinoform focusing units (KL1) and (KL2). Each unit hosts Si wafers with various lenses for different energies and the units provide a travel range along the beam direction to make the focusing more achromatic. For typical SAXS experiments, KL1 is used for horizontal focusing, whereas in WAXS experiments KL1 is used for vertical focusing and KL2 for horizontal focusing.

Experimental Apparatus

The CHX endstation provides a flexible instrument optimized for coherent X-ray scattering studies in SAXS or WAXS geometries, including the possibility of achieving grazing incidence (GI) on liquid samples for GI-SAXS/WAXS. This combination is of particular interest for studies of complex materials and understanding the interplay between structure and dynamics. The endstation features an optics table hosting several beam defining optics, a versatile diffractometer providing both horizontal and vertical scattering geometries and a SAXS table with adjustable flight tube length (up to 15 m).

Computer System

Beamline control is achieved from EPICS via the "Control System Studio" (CSS) which is a set of graphic users interfaces allowing to control each instrument, or "ophyd", a python-based ("spec-like") command line interface for scanning. Data analysis is performed in python with tools provided for standard XPCS analysis.

Current Capabilities Available for Users (as of 1 May 2017)

- X-ray Photon Correlation Spectroscopy
- Coherent Small-Angle X-ray Scattering
- Coherent Wide Angle X-ray Scattering (c-WAXS)

Beamline Specifications

Source Type	Energy Range	Wavelength range	Flux	Focused beam size	Resolution	Technical Quality Metric

IVU20	6-15 keV	λ=2.07-0.83 Å	≈ 2 x 10^{11} p/s (Coherent)	~10 x 10 µm (for SAXS); ~1 x 3 (vxh) µm (for WAXS)	~ 10^{-4}	1

Names of Beamline Personnel and Fractional* FTEs in FY2016

CHX Operations		
YUGANG	ZHANG	1.09
LUTZ	WIEGART	1.02
ANDREI	FLUERASU	1.01
JOE	SULLIVAN	0.52
DAVID	LEVY	0.37
STEPHEN	ANTONELLI	0.32
LEO	REFFI	0.24
RICHARD	GREENE	0.24
WAYNE	LEWIS	0.21
KENNETH	HARSCH	0.10
CHRIS	STELMACH	0.10
MARY	CARLUCCIDAYTON	0.09
GARY	PAPPAS	0.09
SUSAN	MALDONADO	0.07
	MAGILLIII	0.06
JAMES	BIANCAROSA	0.05
59 other staff members contributed effort		1.16
Total		6.73

*Note: 1.0 FTE based on 1760 hours of work. Some staff may log more hours annually

Funding source and fraction of funding for each source FY15-16

FY 2015: DOE – BES; 100%
FY 2016: DOE – BES; 100%
FY 2017: DOE – BES; 100%

Operating funds FY15-16 (K$)

Fiscal Year	Labor Costs	Contract Milestone Payments	Travel	Contract Labor, JT Appts & Shops	Maint/Svc Contracts	Materials & Purchasing	Total Cost

2015	1,362K	110K	16K	252K	69K	267K	2,077K
2016	1,465K	0	2K	109K	46K	273K	1,895K

Allocation Percentages

Fiscal Year**	Maintenance & Start up	General Users	Partner Users	Facility Staff
2015	95.5	4.5	0	0
2016	40.3	55.6	0	4.1
2017	40.3	55.6	0	4.1

** Partial year for 2017.

Number of unique beamline users each year

Fiscal Year**	General Users	Partner Users	Facility Staff	Total
2015	8	0	5	13
2016	32	0	5	37
2017	36	0	5	41

** Partial year for 2017.

Publications: (all publications used NSLS-II photons; numbers in parentheses indicates staff co-authorship)

Calendar Year**	Refereed	DOE High Profile	DOE High Impact	All Publications
2015	0 (0)	0 (0)	0 (0)	0 (0)
2016	1 (1)	0 (0)	0 (0)	2 (1)
2017	0 (0)	0 (0)	0 (0)	0 (0)

** Partial year for 2017.

Complete List of Publications for CY15-17

(includes publications that used NSLS-II photons, beamline R&D publications by staff, and staff research publications; red text indicates publications that used NSLS-II photons)

Refereed Journal Publications

- A Rahman, P Majewski, G Doerk, C Black, K Yager, Non-native Three-dimensional Block Copolymer Morphologies, Nat. Commun., 7, 13988 (2016).
- A Nogales, A Fluerasu, X Ray Photon Correlation Spectroscopy for the Study of Polymer Dynamics, Eur. Polym. J., 81, 494-504 (2016).
- J Rodriguez, R Xu, C Chen, Z Huang, H Jiang, A Chen, K Raines, A Pryor Jr, L Wiegart, et al., Three-dimensional Coherent X-ray Diffractive Imaging of Whole Frozen-hydrated Cells, IUCrJ, 2, 575-583 (2015).

Refereed Conference Proceedings

- L Wiegart, A Fluerasu, D Bruhwiler, O Chubar, Partially Coherent Wavefront Propagation Simulations: Mirror and Monochromator Crystal Quality Assessment, 12th International Conference On Synchrotron Radiation Instrumentation (SRI2015), Vol 1741, p. 040013, sponsored by SRI2015 (2016).
- S Abeykoon, Y Zhang, T Caswell, D Allan, A Akilic, L Wiegart, K Kleese van Dam, A Heroux, M Sutton, Fluerasu et al., Software Tools for X-ray Photon Correlation Spectroscopy and X-ray Speckle Visibility Spectroscopy, 2016 New York Scientific Data Summit (NYSDS), p. 10, sponsored by IEEE, BNL, SUNY at Stony Brook (2016).

Other Publications (books, theses, etc)

- A Madsen, A Fluerasu, B Rutta, Structural Dynamics of Materials Probed by X-Ray Photon Correlation Spectroscopy, Synchrotron Light Sources and Free-Electron Lasers, p. 1-21, Springer International Publishing, Chambery (2016).

12-ID Soft Matter Interfaces (SMI)

Beamline Status

Commissioning

Overall Description

Scientific Scope

Structure and assembly; nano to meso scale; energy and environment.

Beamline Description

The Soft Matter Interfaces beamline will provide Grazing-Incidence SAXS/WAXS and Liquid Interface x-ray scattering capabilities with energy range 2.1-24 keV. SMI is part of the NEXT project and is scheduled for commissioning in September 2016.

Optical System

Separate H and V Mirror focus over entire energy range. Refractive focus tbd. Primary focus at Liquid Spectrometer or at GISAXS sample in low divergence mode or microfocus mode with additional optics.

Experimental Apparatus

Sample vacuum and environmental chamber; Microfluidics; Langmuir troughs; custom user systems.

Computer System

Controls: Linux PC. User support: Windows 7 PC.

Current Capabilities Available for Users (as of 1 May 2017)

- Time-resolved GISAXS/WAXS for samples in vacuum in the 6.5-24 keV energy range, low divergence mode
- Time-resolved GISAXS/WAXS for samples in vacuum in the tender x-ray range, 2.1-6.5 keV, low divergence mode

Beamline Specifications

Source Type	Energy Range	Wavelength range	Flux	Focused beam size	Resolution	Technical Quality Metric
IVU23	2.1 - 24 KeV	5.9 to 0.5 \AA	≈ 10^{13} p/s	2.5(v) x 25(h) µm2	Si (111) VDCM	1

Names of Beamline Personnel and Fractional* FTEs in FY2016

SIX Operations		
WILLIAM	OBRIEN	0.06
MICHAEL	BROMFIELD	0.05
8 other staff members contributed effort		0.12
Total		0.23

*Note: 1.0 FTE based on 1760 hours of work. Some staff may log more hours annually

Funding source and fraction of funding for each source FY15-16

FY 2015: DOE – BES; 100%
FY 2016: DOE – BES; 100%
FY 2017: DOE – BES; 100%

Operating funds FY15-16 (K$)

Fiscal Year	Labor Costs	Contract Milestone Payments	Travel	Contract Labor, JT Appts & Shops	Maint/Svc Contracts	Materials & Purchasing	Total Cost
2015	n/a	n/a	n/a	n/a	n/a	n/a	n/a
2016	9K		13K			11K	33K

Allocation Percentages

Fiscal Year**	Maintenance & Start up	General Users	Partner Users	Facility Staff
2015	n/a	n/a	n/a	n/a
2016	n/a	n/a	n/a	n/a
2017	60	36	0	4

** Partial year for 2017.

Number of unique beamline users each year

Fiscal Year**	General Users	Partner Users	Facility Staff	Total
2015	n/a	n/a	n/a	n/a
2016	n/a	n/a	n/a	n/a
2017	6	0	5	11

** Partial year for 2017.

Publications: (all publications used NSLS-II photons; numbers in parentheses indicates staff co-authorship)

Calendar Year**	Refereed	DOE High Profile	DOE High Impact	All Publications
2015	n/a	n/a	n/a	n/a
2016	n/a	n/a	n/a	n/a
2017	n/a	n/a	n/a	n/a

** Partial year for 2017.

Complete List of Publications for CY15-17

(includes publications that used NSLS-II photons, beamline R&D publications by staff, and staff research publications; red text indicates publications that used NSLS-II photons)

Refereed Journal Publications

- M Zhernenkov, D Bolmatov, D Soloviov, K Zhernenkov, B Toperverg, A Cunsolo, A Bosak, Y Cai, Revealing the Mechanism of Passive Transport in Lipid Bilayers via Phonon-mediated Nanometre-scale Density Fluctuations, Nat. Commun., 7, 11575 (2016). [108276]
- D Bolmatov, M Zhernenkov, D Zav'yalov, S Stoupin, A Cunsolo, Y Cai, Thermally Triggered Phononic Gaps in Liquids at THz Scale, Sci. Rep., 6, 19469 (2016). [108070]
- D Bolmatov, M Zhernenkov, D Zav'yalov, Y Cai, A Cunsolo, Terasonic Excitations in 2D Gold Nanoparticle Arrays in a Water Matrix as Revealed by Atomistic Simulations, J. Phys. Chem. C, 120(35), 19896–19903 (2016). [112690]
- S Stoupin, M Zhernenkov, B Shi, Surface Studies of Solids Using Integral X-ray-induced Photoemission Yield, Sci. Rep., 5, 37440 (2016). [113259]

- D Bolmatov, M Zhernenkov, D Zav'yalov, S Tkachev, A Cunsolo, Y Cai, The Frenkel Line: a Direct Experimental Evidence for the New Thermodynamic Boundary, Sci. Rep., 5, 15850 (2015). [107811]
- M Zhernenkov, R Ashkar, H Feng, O Akintewe, N Gallant, R Toomey, J Ankner, R Pynn, Thermoresponsive PNIPAM Coatings on Nanostructured Gratings for Cell Alignment and Release, ACS Appl. Mater. Interfaces, 7(22), 11857–11862 (2015). [107810]
- D Bolmatov, M Zhernenkov, D Zav'yalov, S Stoupin, Y Cai, A Cunsolo, Revealing the Mechanism of the Viscous-to-Elastic Crossover in Liquids, J. Phys. Chem. Letts., 6(15), 3048–3053 (2015). [108218]
- D Bolmatov, D Zav'yalov, M Zhernenkov, E Musaev, Y Cai, Unified Phonon-based Spproach to the Thermodynamics of Solid, Liquid and Gas States, 363, 221-242 (2015).

16-ID Life Science X-ray Scattering (LIX)

Beamline Status

Operations

Overall Description

Scientific Scope

Structure of macromolecules in solution; Scattering-based imaging of biological tissues; Membrane structures

Beamline Description

This is a x-ray scattering beamline designed specifically for life science applications.

Optical System

White beam mirror (flat); Si(111) monochromator (channel cut + fixed-exit pair); KB focusing mirrors; Secondary focusing beryllium lenses

Experimental Apparatus

Automatic sample handler for solution scattering. Scanning microscope stage for in-air imaging and scattering measurements.

Computer System

Workstations for beamline control. Linux cluster for data analysis and storage.

Current Capabilities Available for Users (as of 1 May 2017)

- Static solution scattering
- Solution scattering with in-line size exclusion chromatography
- micro-beam diffraction with a beam size of 5 micron or smaller

Beamline Specifications

Source Type	Energy Range	Wavelength range	Flux	Focused beam size	Resolution	Technical Quality Metric
IVU23	2.1-18 KeV	5.9 - 0.69 Å	$\approx 10^{13}$ p/s	1μm	$\sim 10^{-4}$	1

Names of Beamline Personnel and Fractional* FTEs in FY2016

LIX Operations		
KUN	QIAN	0.34
VITO	GRAZIANO	0.34
JOHN	SKINNER	0.34
ALEXEI	SOARES	0.33
EDWIN	LAZO	0.33
JEAN	JAKONCIC	0.31
BOB	SWEET	0.27
LIN	YANG	0.24
SHIRISH	CHODANKA	0.24
HUGO	SLEPICKA	0.24
GRACE	SHEAMCCA	0.23
JONATHAN	DIFABIO	0.23
SEAN	MCSWEEN	0.19
BABAK	ANDI	0.18
VIVIAN	STOJANOF	0.18
JOHN	LARA	0.15
MATT	COWAN	0.15
MARTIN	FUCHS	0.14
RICHARD	JACKIMOW	0.13
DIETER	SCHNEIDER	0.13
CORNELIUS	WHALEN	0.12
DILEEP	BHOGADI	0.11
NICOLAS	GUICHARD	0.11
THOMAS	LANGDON	0.08
BRUNO	SEIVAMART	0.08
STUART	MYERS	0.06
8 other staff efforts		0.20
Total		5.47

*Note: 1.0 FTE based on 1760 hours of work. Some staff may log more hours annually

Funding source and fraction of funding for each source FY15-16

FY 2015: DOE – BER/NIH; 50%/50%
FY 2016: DOE – BER/NIH; 50%/50%
FY 2017: DOE – BER/NIH; 50%/50%

Operating funds FY15-16 (K$)

Fiscal Year	Labor Costs	Contract Milestone Payments	Travel	Contract Labor, JT Appts & Shops	Maint/Svc Contracts	Materials & Purchasing	Total Cost
2015	n/a	n/a	n/a	n/a	n/a	n/a	n/a
2016	n/a	n/a	n/a	n/a	n/a	n/a	n/a

Allocation Percentages

Fiscal Year**	Maintenance & Start up	General Users	Partner Users	Facility Staff
2015	n/a	n/a	n/a	n/a
2016	97.9	1.3	0	0.8
2017	63	36	0	7

** Partial year for 2017.

Number of unique beamline users each year

Fiscal Year**	General Users	Partner Users	Facility Staff	Total
2015	n/a	n/a	n/a	n/a
2016	6	0	6	12
2017	49	0	3	52

** Partial year for 2017.

Publications: (all publications used NSLS-II photons; numbers in parentheses indicates staff co-authorship)

Calendar Year**	Refereed	DOE High Profile	DOE High Impact	All Publications
2015	n/a	n/a	n/a	n/a
2016	0 (0)	0 (0)	0 (0)	0 (0)
2017	0 (0)	0 (0)	0 (0)	0 (0)

** Partial year for 2017.

Complete List of Publications for CY15-17

(includes publications that used NSLS-II photons, beamline R&D publications by staff, and staff research publications; red text indicates publications that used NSLS-II photons)

Refereed Journal Publications

- L Song, L Yang, J Meng, S Yang, Thermodynamics of Hydrophobic Amino Acids in Solution: A Combined Experimental–Computational Study, J. Phys. Chem. Lett, 8, 347–351 (2017).
- J Kim, J Kim, S Jo, J Kang, J Jo, M Lee, J Moon, L Yang, M Kim, et al., Ultrahigh Detective Heterogeneous Photosensor Arrays with In-Pixel Signal Boosting Capability for Large-Area and Skin-Compatible Electronics, Adv. Mats., 28, 3078-3086 (2016).
- M Fukuto, L Yang, D Nykypanchuk, I Kuzmenko, Transmission X-ray Scattering as a Probe for Complex Liquid-surface Structures, J. Synch. Rad., 23, 519-531 (2016). [108469]
- K Nygard, S Sarman, K Hyltegren, S Chodankar, E Perret, J Buitenhuis, J van der Veen, R Kjellander, Density Fluctuations of Hard-Sphere Fluids in Narrow Confinement, Phys. Rev. X, 6(1), 011014 (2016).
- J Kim, M Kim, J Kim, S Jo, J Kang, J Jo, W Lee, C Hwang, L Yang, et al., Scalable Sub-micron Patterning of Organic Materials Toward High Density Soft Electronics, Sci. Rep., 5, 14520 (2015).
- Zhang, H Inouye, L Yang, M Himmel, M Tucker, L Makowski, Breakdown of Hierarchical Architecture in Cellulose During Dilute Acid Pretreatments, Cellulose, 22, 1495-1504 (2015).

Refereed Conference Proceedings

- J DiFabio, S Chodankar, S Pjerov, J Jakoncic, M Lucas, C Krywka, V Graziano, L Yang, The Life Science X-ray Scattering Beamline at NSLS-II, Synchrotron Radiation Instrumentation (SRI 2015), Vol 1741, sponsored by USDOE Office of Science (SC) (2016).
- H Bernstein, B Andi, K Badalian, L Berman, D Bhogadi, S Chodankar, J DiFabio, M Fuchs, J Jakoncic, et al., Computing Infrastructure, Software Optimization, and Real Time Analysis for High Data-rate MX, Scientific Data Summit (NYSDS), 2016 New York, p. 1-4, sponsored by IEEE (2016).

17-BM Footprinting for In Vitro and in Vivo Structural Studies in Biological Macromolecules (XFP)

Beamline Status

Operations

Overall Description

Scientific Scope

X-ray Footprinting for in Vitro and in Vivo Structural Studies of Biological Macromolecules (XFP) is a 3-pole wiggler beamline at 17-BM providing world-leading X-ray Footprinting capabilities for solution state studies of biological macromolecular structure and dynamics. The focused broadband X-ray beam delivers flexible beam spot sizes to adapt to sample configurations; the high flux density of the XFP beam enables achievement of exposure times of less than a millisecond for high quality data on complex samples in physiologically relevant conditions and timescales.

Beamline Description

The XFP beamline is a partner beamline operated by the Case Western Reserve University Center for Synchrotron Biosciences. The beamline delivers high flux density broadband x-rays to several sample exposure positions on separate tables in the experimental hutch. With adjustable focusing of the toroidal mirror longitudinal radius and distance from the source, the beam size can be tailored to a variety of samples. Standard sample exposure is performed using the capillary flow apparatus (recommended 100 uL of sample per exposure). Science commissioning of additional resources for high-throughput, low volume (5 uL) frozen and room temperature experiments, time-resolved flow experiments and in vivo capillary flow experiments is currently ongoing. A sample preparation area is located just downstream of the hutch, containing laboratory equipment required for sensitive sample handling. This beamline is constructed and is being operated in partnership with Case Western Reserve University.

Energy Range:5-16 keV

Flux:10^{15} ph/s; >500 W/mm^2 at focus

Mono Crystal Grating: None

Resolution:broadband

Spot Size:120 um V x 450 um H to 2.6 x 2.6 mm

Total Angular Acceptance:3 mrad H, 0.33 mrad V

Optical System

Front End Toroidal Focusing mirror (Rh coating, 4.2 mrad angle)

Experimental Apparatus

Standard beamline apparatus: Capillary flow cell (direct syringe pump)

In Science Commissioning: High-throughput 23-sample steady state apparatus (-30C - 60C); *In-Vivo* multi-pump system with in-line incubator and fraction collector; Time-resolved apparatus (direct syringe pump driven with turbulent mixer)

Computer System

HP Workstation and IOC server with Debian Linux; running Control System Studio for basic motor controls with scripts for experimental controls systems implemented through ipython (Ophyd/bluesky).

Current Capabilities Available for Users (as of 1 May 2017)

- Steady-state X-ray Footprinting (capillary flow)
- High-throughput (low volume, liquid or frozen state) X-ray Footprinting
- Time-resolved X-ray Footprinting

Beamline Specifications

Source Type	Energy Range	Wavelength range	Flux	Focused beam size	Resolution	Technical Quality Metric
3PW	5-20 KeV	N/A	$\approx 5 \times 10^{16}$ p/s	$\approx 100 \times 500$ μm^2	Pink Beam	1

Names of Beamline Personnel and Fractional* FTEs in FY2016

*Note: 1.0 FTE based on 1760 hours of work. Some staff may log more hours annually

Funding source and fraction of funding for each source FY15-16

FY 2015: Case Western Reserve University; 100%
FY 2016: Case Western Reserve University; 100%
FY 2017: Case Western Reserve University; 100%

Operating funds FY15-16 (K$)

Fiscal Year	Labor Costs	Contract Milestone Payments	Travel	Contract Labor, JT Appts & Shops	Maint/Svc Contracts	Materials & Purchasing	Total Cost
2015	n/a	n/a	n/a	n/a	n/a	n/a	n/a
2016	n/a	n/a	n/a	n/a	n/a	n/a	n/a

Allocation Percentages

Fiscal Year**	Maintenance & Start up	General Users	Partner Users	Facility Staff
2015	n/a	n/a	n/a	n/a
2016	n/a	n/a	n/a	n/a
2017	65	29	3	3

** Partial year for 2017.

Number of unique beamline users each year

Fiscal Year**	General Users	Partner Users	Facility Staff	Total
2015	n/a	n/a	n/a	n/a
2016	3	0	8	11
2017	16	5	0	21

** Partial year for 2017.

Publications: (all publications used NSLS-II photons; numbers in parentheses indicates staff co-authorship)

Calendar Year**	Refereed	DOE High Profile	DOE High Impact	All Publications
2015	n/a	n/a	n/a	n/a
2016	0 (0)	0 (0)	0 (0)	0 (0)
2017	0 (0)	0 (0)	0 (0)	0 (0)

** Partial year for 2017.

Complete List of Publications for CY15-17

(includes publications that used NSLS-II photons, beamline R&D publications by staff, and staff research publications; red text indicates publications that used NSLS-II photons)

Refereed Journal Publications

- R Hulscher, J Bohon, M Rappe, S Gupta, R D'Mello, M Sullivan, C Ralston, M Chance, S Woodson, Probing the Structure of Ribosome Assembly Intermediates in vivo Using DMS and Hydroxyl Radical Footprinting, Methods, 103, 49-56 (2016).
- J Bohon, E Muller, W Ding, M Gaowei, T Zhou, J Smedley, Transmission X-Ray Imaging Detector Captures the Last Light at NSLS, Biophys. J., 108(2), 620a (2015).
- T Zhou, W Ding, M Gaowei, G De Geronimo, J Bohon, J Smedley, E Muller, Pixelated Transmission-mode Diamond X-ray Dector, J. Synch. Rad., 22(6), 1396-1402 (2015).
- Y Zhai, O Baturina, D Ramaker, E Farquhar, J St-Pierre, K Swider-Lyons, Bromomethane Contamination in the Cathode of Proton Exchange Membrane Fuel Cells, Electrochim. Acta, 213, 482-489 (2016).
- R Singh, H Dong, D Liu, L Zhao, A Marts, E Farquhar, D Tierney, C Almquist, B Briggs, Reduction of Hexavalent Chromium by the Thermophilic Methanogen Methanothermobacter Thermautotrophicus, Geochim. Cosmochim. Acta, 148, 442-456 (2015).
- P Pirovano, E Farquhar, M Swart, A Fitzpatrick, G Morgan, A McDonald, Characterization and Reactivity of a Terminal Nickel(III)–Oxygen Adduct, Chem. Eur. J., 21(9), 3785-3790 (2015).
- W Nettles, H Song, E Farquhar, N Fitzkee, J Emerson, Characterization of the Copper(II) Binding Sites in Human Carbonic Anhydrase II, Inorg. Chem., 54(12), 5671-5680 (2015).
- Y Zhai, O Baturina, D Ramaker, E Farquhar, J St-Pierre, K Swider-Lyons, Chlorobenzene Poisoning and Recovery of Platinum-Based Cathodes in Proton Exchange Membrane Fuel Cells, J. Phys. Chem. C, 119(35), 20328-20338 (2015).

Refereed Conference Proceedings

- J Bohon, M Sullivan, J Dvorak, D Abel, J Toomey, M Chance, Development of the XFP Beamline for X-ray Footprinting at NSLS-II, 12th International Conference on Synchrotron Radiation Instrumentation, Vol 1741, p. 030005, sponsored by Brookhaven National Laboratory (2016).
- J Bohon, M Sullivan, J Dvorak, D Abel, J Toomey, M Chance, Development of the XFP Beamline for X-ray Footprinting at NSLS-II, AIP Conference Proceedings, Vol 1741, p. 030005, sponsored by AIP Conf. Proc. (2016).

17-ID-1 Highly Automated Macromolecular Crystallography Beamline (AMX)

Beamline Status

Operations

Overall Description

Scientific Scope

AMX is a highly automated macromolecular crystallography beamline designed to meet the needs of the biomedical researcher in revealing structure and function of living systems. With its best in class high-flux mini beam of 4 µm size and low divergence, and with its readily available larger beams to 100 µm, it supports data collections at cryogenic and room temperatures, in crystallization media, and by serial crystallography methods. Its high flux, fast framing detector, and automated sample exchange robotics enable investigators to efficiently discover the best diffracting crystal among available specimen, to carry out exhaustive binding studies, and to collect highly redundant data sets from many crystals to find by hierarchical sorting the conformers and classes that yield the highest resolution structures. AMX supports the visiting scientist, the remote participant, and is capable of database-driven automatic data collections.

Beamline Description

AMX, part of the NIH-funded ABBIX construction project, is a highly automated macromolecular crystallography beamline with best in class flux among the mini-beam lines. Its capabilities overlap and complement those of the FMX micro-diffraction macromolecular crystallography with which it shares sector 17-ID.

Optical System

White beam slits, double crystal Si (111) monochromator with horizontal theta-axis, tandem flat beam deflecting silicon mirrors (Pd and Si lanes), Kirkpatrick-Baez focusing silica mirrors, Pd coated, each bent adaptively with 16 piezo actuators. Each optical element is preceded by slits and its transmitted beam is monitored by beam position monitors or retractable screens.

Experimental Apparatus

High-precision horizontal axis goniometer for data collection from cryogenic specimen, exchangeable with a secondary goniometer for data collection at room temperature from specimen in crystallization plates, on-axis reflective optics microscope, dynamical beam shaping slits, six-axis sample changing robot with high capacity specimen dewar, Pilatus 6M pixel-array detector framing at up to 25 Hz.

Computer System

Pilatus processing unit for Bragg spot finding and local data buffering; high speed network to transmit data to a central compute cluster and disk farm for data reduction and structure solving; separate software servers for beamline device control, configuration archiving, and experiment control, database, and crystallographic software; several user workstations.

Current Capabilities Available for Users (as of 1 May 2017)

Macromolecular crystallography with a beam size of 5 – 100 µm, an energy range of 5 – 18 keV, automatic specimen handling, and data collection with an Eiger X 9M detector at framing rates up to 238 Hz.

Beamline Specifications

Source Type	Energy Range	Wavelength range	Flux	Focused beam size	Resolution	Technical Quality Metric
IVU21	5 – 18 keV	0.7 – 2.5 Å	≈ $2x10^{13}$ p/s	min: 4 µm x 3 µm range: 5–100 µm	real space: 1.5 - 1000 Å	1

Names of Beamline Personnel and Fractional* FTEs in FY2016

AMX Operations		
KUN	QIAN	0.34
VITO	GRAZIANO	0.34
JOHN	SKINNER	0.34
ALEXEI	SOARES	0.33
EDWIN	LAZO	0.33
JEAN	JAKONCIC	0.31
BOB	SWEET	0.27
LIN	YANG	0.24
SHIRISH	CHODANKA	0.24
HUGO	SLEPICKA	0.24
GRACE	SHEAMCCA	0.23
JONATHAN	DIFABIO	0.23
SEAN	MCSWEEN	0.19
BABAK	ANDI	0.18
VIVIAN	STOJANOF	0.18
JOHN	LARA	0.15
MATT	COWAN	0.15
MARTIN	FUCHS	0.14
RICHARD	JACKIMOW	0.13
DIETER	SCHNEIDER	0.13
CORNELIUS	WHALEN	0.12
DILEEP	BHOGADI	0.11
NICOLAS	GUICHARD	0.11
THOMAS	LANGDON	0.08
BRUNO	SEIVAMARI	0.08
STUART	MYERS	0.06
8 other staff efforts		0.20
Total		5.47

*Note: 1.0 FTE based on 1760 hours of work. Some staff may log more hours annually

Funding source and fraction of funding for each source FY15-16

FY 2015: DOE – BER/NIH; 50%/50%
FY 2016: DOE – BER/NIH; 50%/50%
FY 2017: DOE – BER/NIH; 50%/50%

Operating funds FY15-16 (K$)

Fiscal Year	Labor Costs	Contract Milestone Payments	Travel	Contract Labor, JT Appts & Shops	Maint/Svc Contracts	Materials & Purchasing	Total Cost
2015	n/a	n/a	n/a	n/a	n/a	n/a	n/a
2016	n/a	n/a	n/a	n/a	n/a	n/a	n/a

Allocation Percentages

Fiscal Year**	Maintenance & Start up	General Users	Partner Users	Facility Staff
2015	n/a	n/a	n/a	n/a
2016	99.4	0.6	0	0
2017	77	21	0	2

** Partial year for 2017.

Number of unique beamline users each year

Fiscal Year**	General Users	Partner Users	Facility Staff	Total
2015	n/a	n/a	n/a	n/a
2016	3	0	11	14
2017	2	0	0	2

** Partial year for 2017.

Publications: (all publications used NSLS-II photons; numbers in parentheses indicates staff co-authorship)

Calendar Year**	Refereed	DOE High Profile	DOE High Impact	All Publications
2015	n/a	n/a	n/a	n/a
2016	0 (0)	0 (0)	0 (0)	0 (0)
2017	0 (0)	0 (0)	0 (0)	0 (0)

** Partial year for 2017.

Complete List of Publications for CY15-17

(includes publications that used NSLS-II photons, beamline R&D publications by staff, and staff research publications; red text indicates publications that used NSLS-II photons)

Refereed Conference Proceedings

- M Fuchs, D Bhogadi, J Jakoncic, S Myers, R Sweet, L Berman, J Skinner, M Idir, O Chubar, et al., NSLS-II Biomedical Beamlines for Micro-crystallography, FMX, and for Highly Automated Crystallography, AMX: New Opportunities for Advanced Data Collection, 12th International Conference on Synchrotron Radiation Instrumentation - SRI2015, Vol 1741, p. 030006, sponsored by National Synchrotron Light Source II (2016).
- H Bernstein, B Andi, K Badalian, L Berman, D Bhogadi, S Chodankar, J DiFabio, M Fuchs, J Jakoncic, et al., Computing Infrastructure, Software Optimization, and Real Time Analysis for High Data-rate MX, Scientific Data Summit (NYSDS), 2016 New York, p. 1-4, sponsored by IEEE (2016).

17-ID-2 Frontier Microfocusing Macromolecular Crystallography (FMX)

Beamline Status

Operations

Overall Description

Scientific Scope

Frontier macromolecular crystallography (FMX) is an undulator beamline at sector 17-ID for structural biology investigations with micro-focusing macromolecular crystallography (MX), optimized for challenging bio-crystallographic problems. Its flux density is unmatched by MX facilities worldwide.

Beamline Description

The FMX beamline is operated through the NIH-funded Life Science and Biological Research resource. It supports micro-focus macromolecular crystallography, serial crystallography, and data collection at cryo- and room temperature.

Optical System

Double crystal monochromator (vertical axis, Si 111) > Horizontally focusing bimorph mirror < Horizontal secondary source > Focusing compound refractive lenses > KB focusing bimorph mirrors.

Experimental Apparatus

Robotic sample mounting; Dectris Eiger 16M area detector (data rate 133 Hz at full frame, 750 Hz in 4M region); 100 nm precision main goniometer; high resolution sample viewing microscope with intrinsic fluorescence imaging.

Computer System

Integrated Graphical User Interface LSDC with Python scripting facility. Beamline control through EPICS. Parallelized ata processing pipeline on high-performance computing cluster dedicated for data processing and automated structure solution.

Current Capabilities Available for Users (as of 1 May 2017)

Macromolecular micro-crystallography with a beam size of 1 x 1.5 µm^2, an energy range from 5-30 keV, and sample mounting automation. The Eiger 16M detector supports rapid data collection at rates of 133 Hz for a full frame and 750 Hz for a 4M region.

Beamline Specifications

Source Type	Energy Range	Wavelength range	Flux	Focused beam size	Resolution	Technical Quality Metric
IVU21	5-30 keV	0.4 - 2.5 Å	~ 10^{13} p/s	min: 1 µm x 1 µm range: 1 - 20 µm	real space: 1.5 - 1000 Å	1

Names of Beamline Personnel and Fractional* FTEs in FY2016

FMX Operations		
KUN	QIAN	0.34
VITO	GRAZIANO	0.34
JOHN	SKINNER	0.34
ALEXEI	SOARES	0.33
EDWIN	LAZO	0.33
JEAN	JAKONCIC	0.31
BOB	SWEET	0.27
LIN	YANG	0.24
SHIRISH	CHODANKA	0.24
HUGO	SLEPICKA	0.24
GRACE	SHEAMCCA	0.23
JONATHAN	DIFABIO	0.23
SEAN	MCSWEEN	0.19
BABAK	ANDI	0.18
VIVIAN	STOJANOF	0.18
JOHN	LARA	0.15
MATT	COWAN	0.15
MARTIN	FUCHS	0.14
RICHARD	JACKIMOW	0.13
DIETER	SCHNEIDER	0.13
CORNELIUS	WHALEN	0.12
DILEEP	BHOGADI	0.11
NICOLAS	GUICHARD	0.11
THOMAS	LANGDON	0.08
BRUNO	SEIVAMAR	0.08
STUART	MYERS	0.06
8 other staff efforts		0.20
Total		5.47

*Note: 1.0 FTE based on 1760 hours of work. Some staff may log more hours annually

Funding source and fraction of funding for each source FY15-16

FY 2015: DOE – BER/NIH; 50%/50%
FY 2016: DOE – BER/NIH; 50%/50%
FY 2017: DOE – BER/NIH; 50%/50%

Operating funds FY15-16 (K$)

Fiscal Year	Labor Costs	Contract Milestone Payments	Travel	Contract Labor, JT Appts & Shops	Maint/Svc Contracts	Materials & Purchasing	Total Cost
2015	n/a	n/a	n/a	n/a	n/a	n/a	n/a
2016	n/a	n/a	n/a	n/a	n/a	n/a	n/a

Allocation Percentages

Fiscal Year**	Maintenance & Start up	General Users	Partner Users	Facility Staff
2015	n/a	n/a	n/a	n/a
2016	99.4	0.6	0	0
2017	80	18	0	2

** Partial year for 2017.

Number of unique beamline users each year

Fiscal Year**	General Users	Partner Users	Facility Staff	Total
2015	n/a	n/a	n/a	n/a
2016	12	0	11	23
2017	32	1	17	50

** Partial year for 2017.

Publications: (all publications used NSLS-II photons; numbers in parentheses indicates staff co-authorship)

Calendar Year**	Refereed	DOE High Profile	DOE High Impact	All Publications
2015	n/a	n/a	n/a	n/a
2016	0 (0)	0 (0)	0 (0)	0 (0)
2017	0 (0)	0 (0)	0 (0)	0 (0)

** Partial year for 2017.

Complete List of Publications for CY15-17

(includes publications that used NSLS-II photons, beamline R&D publications by staff, and staff research publications; red text indicates publications that used NSLS-II photons)

Refereed Journal Publications

- R Owen, J Juanhuix, M Fuchs, Current Advances in Synchrotron Radiation Instrumentation for MX Experiments, Arch. Biochem. Biophys., 602, 21-31 (2016). [112616]
- S Waltersperger, V Olieric, C Pradervand, W Glettig, M Salathe, M Fuchs, A Curtin, X Wang, S Ebner, et al., PRIGo: A New Multi-axis Goniometer for Macromolecular Crystallography, J. Synch. Rad., 22(4), 895-900 (2015).
- F Dworkowski, M Hough, G Pompidor, M Fuchs, Challenges and Solutions for the Analysis of In Situ, in Crystallo Micro-spectrophotometric Data, Acta Cryst. D, D71, 27-35 (2015). [107352]

Refereed Conference Proceedings

- M Fuchs, D Bhogadi, J Jakoncic, S Myers, R Sweet, L Berman, J Skinner, M Idir, O Chubar, et al., NSLS-II Biomedical Beamlines for Micro-crystallography, FMX, and for Highly Automated Crystallography, AMX: New Opportunities for Advanced Data Collection, 12th International Conference on Synchrotron Radiation Instrumentation - SRI2015, Vol 1741, p. 030006, sponsored by National Synchrotron Light Source II (2016).
- H Bernstein, B Andi, K Badalian, L Berman, D Bhogadi, S Chodankar, J DiFabio, M Fuchs, J Jakoncic, et al., Computing Infrastructure, Software Optimization, and Real Time Analysis for High Data-rate MX, Scientific Data Summit (NYSDS), 2016 New York, p. 1-4, sponsored by IEEE (2016).

18-ID Full Field X-ray Imaging (FXI)

Beamline Status

Construction

Overall Description

Scientific Scope

3D in-situ and in-operando dynamics of sample morphology and oxidation states imaged at 30 nm spatial resolution. Scientific areas include energy storage devices, materials science and environmental science.

Description

FXI will house a Transmission X-ray Microscope (TXM) with 30 nm spatial resolution and 20-40 micron field of view. At 500 mA NSLS-II operation, the expected exposure time per image is < 100 ms. The TXM is also capable of nanoXANES, which will allow for the identification of chemical states of some elements. The FXI beamline is in the contingency scope of the NEXT project.

Optical System

Collimating mirror - DCM - Toroidal mirror. Energy bandwidth is Si(111) or ~ 1.4 x 10-4. Toroidal mirror focuses beam onto a secondary source (~ 260 um H x 240 um V) about 2 m upstream of the TXM. The TXM condenser will focus the secondary source to about 12-14 um spot on the sample. Condenser agitation or a beam disperser will increase the focus size on the sample to ~ 20-40 um field of view.

Experimental Apparatus

Transmission X-ray Microscope (XRADIA). 30 nm spatial resolution. 20-40 micron field of view. Some in-situ sample environmental cells are available.

Computer System

Proprietary XRADIA controls software

Current Capabilities Available for Users (as of 1 May 2017)

N/A

Beamline Specifications

Source Type	Energy Range	Wavelength range	Flux	Focused beam size	Resolution	Technical Quality Metric
DW100	5-11 KeV		≈ 10^{13} p/s on sample	20-40 um (FOV)	30 nm spatial; < 50 ms exposure time per image	1

Names of Beamline Personnel and Fractional* FTEs in FY2016

Note: 1.0 FTE based on 1760 hours of work. Some staff may log more hours annually

Funding source and fraction of funding for each source FY15-16

FY 2015: DOE – BES; 100%
FY 2016: DOE – BES; 100%
FY 2017: DOE – BES; 100%

Operating funds FY15-16 (K$)

Fiscal Year	Labor Costs	Contract Milestone Payments	Travel	Contract Labor, JT Appts & Shops	Maint/Svc Contracts	Materials & Purchasing	Total Cost
2015	n/a	n/a	n/a	n/a	n/a	n/a	n/a
2016	n/a	n/a	n/a	n/a	n/a	n/a	n/a

Allocation Percentages

Fiscal Year**	Maintenance & Start up	General Users	Partner Users	Facility Staff
2015	n/a	n/a	n/a	n/a
2016	n/a	n/a	n/a	n/a
2017	n/a	n/a	n/a	n/a

** Partial year for 2017.

Number of unique beamline users each year

Fiscal Year**	General Users	Partner Users	Facility Staff	Total
2015	n/a	n/a	n/a	n/a
2016	n/a	n/a	n/a	n/a
2017	n/a	n/a	n/a	n/a

** Partial year for 2017.

Publications: (all publications used NSLS-II photons; numbers in parentheses indicates staff co-authorship)

Calendar Year**	Refereed	DOE High Profile	DOE High Impact	All Publications
2015	n/a	n/a	n/a	n/a
2016	n/a	n/a	n/a	n/a
2017	n/a	n/a	n/a	n/a

** Partial year for 2017.

Complete List of Publications for CY15-17

(includes publications that used NSLS-II photons, beamline R&D publications by staff, and staff research publications; red text indicates publications that used NSLS-II photons)

Refereed Journal Publications

- S Imhott, P Gibbs, M Katz, T Ott Jr., B Patterson, W K. Lee, K Fezzaa, J Cooley, A Clarke, Dynamic Evolution of Liquid-liquid Phase Separation During Continuous Cooling, Mater. Chem. Phys., 153, 93-102 (2015).

Refereed Conference Proceedings

- W Lee, R Reininger, W Loo, R Gambella, S O'Hara, Y Chu, Z Zhong, J Wang, FXI: A Full-field Imaging Beamline at NSLS-II, X-Ray Nanoimaging: Instruments and Methods II, 959209 , Vol 9592, sponsored by Barry Lai (2015).

19-ID Biological Microdiffraction Facility (NYX)

Beamline Status

Commissioning

Overall Description

Scientific Scope

While moving to incorporate microbeams, we also want to preserve the versatility of optimized anomalous scattering experiments across a broad spectrum of atomic resonances from different elements and we propose to capitalize on the intrinsic brightness of NSLS-II to optimize anomalous signals by improving energy resolution.

Beamline Description

This beamline has the scientific objective of providing a state-of-the-art source for a wide spectrum of crystallographic experiments and a cutting-edge source for optimized anomalous diffraction experiments. This beamline is constructed and will be operated in partnership with the New York Structural Biology Consortium (NYSBC).

Optical System

Double crystal monochrometer, focusing mirror

Experimental Apparatus

Crystal Logic microdiffractometer

Computer System

Stanford Blu-Ice

Current Capabilities Available for Users (as of 1 May 2017)

N/A

Beamline Specifications

Source Type	Energy Range	Wavelength range	Flux	Focused beam size	Resolution	Technical Quality Metric
IVU20	3.5-17 KeV					

Names of Beamline Personnel and Fractional* FTEs in FY2016

*Note: 1.0 FTE based on 1760 hours of work. Some staff may log more hours annually

Funding source and fraction of funding for each source FY15-16

FY 2015: New York Structural Biology Center; 100%
FY 2016: New York Structural Biology Center; 100%
FY 2017: New York Structural Biology Center; 100%

Operating funds FY15-16 (K$)

Fiscal Year	Labor Costs	Contract Milestone Payments	Travel	Contract Labor, JT Appts & Shops	Maint/Svc Contracts	Materials & Purchasing	Total Cost
2015	n/a	n/a	n/a	n/a	n/a	n/a	n/a
2016	n/a	n/a	n/a	n/a	n/a	n/a	n/a

Allocation Percentages

Fiscal Year**	Maintenance & Start up	General Users	Partner Users	Facility Staff
2015	n/a	n/a	n/a	n/a
2016	n/a	n/a	n/a	n/a
2017	n/a	n/a	n/a	n/a

** Partial year for 2017.

Number of unique beamline users each year

Fiscal Year**	General Users	Partner Users	Facility Staff	Total
2015	n/a	n/a	n/a	n/a
2016	n/a	n/a	n/a	n/a
2017	n/a	n/a	n/a	n/a

** Partial year for 2017.

Publications: (all publications used NSLS-II photons; numbers in parentheses indicates staff co-authorship)

Calendar Year**	Refereed	DOE High Profile	DOE High Impact	All Publications
2015	n/a	n/a	n/a	n/a
2016	n/a	n/a	n/a	n/a
2017	n/a	n/a	n/a	n/a

** Partial year for 2017.

Complete List of Publications for CY15-17

(includes publications that used NSLS-II photons, beamline R&D publications by staff, and staff research publications; red text indicates publications that used NSLS-II photons)

Refereed Journal Publications

Refereed Conference Proceedings

Other Publications (books, theses, etc)

21-ID Electron Spectro-Microscopy (ESM)

Beamline Status

Commissioning

Overall Description

Scientific Scope

The experimental study of the novel materials - often artificially engineered - is the fundamental scientific scope of the ESM beamline. The beamline feeds two photoemission end stations. Branch 1) is a high resolution SP-ARPES spectrometer and branch 2) is a full-field AC-XPEEM/LEEM instrument (in collaboration with the BNL Center for Functional Nanomaterials).

Beamline Description

ESM is a soft X-ray beamline optimized for high-resolution photoemission microscopy. Two branches: μ-SARPES, XPEEM

Optical System

Monochromator (VLS-PGM). Secondary slits. μ-ARPES refocusing: KB pair; XPEEM-refocusing: ellipsoidal.

Experimental Apparatus

μ-SARPES

• Smaract micro-scanning stage • Scienta DA30 with 2D mini-Mott • Closed cycle LHe cryostats.

XPEEM branch:

• Elmitec AC-LEEM III (Aberration-Corrected Low Energy Electron Microscope)

Computer System

Beamline components are controlled by EPICS 3.14 using VME. The user interface is through Python and Control System Studio (CSS) clients.

Current Capabilities Available for Users (as of 1 May 2017)

- Photoemission (ARPES, XPS) and absorption (XAS) with a photon energy of 250 - 1500 eV, spot size of 50 microns, sample temperature range from 30 – 1000 K, and the Scienta DA30 electron energy analyzer.

- X-ray photoemission electron microscopy (XPEEM) with ~10nm spatial resolution; chemical, electronic and topographic imaging at nanometer scale; micro-spot spectroscopy; micro-spot low energy electron diffraction.

Beamline Specifications

Source Type	Energy Range	Wavelength range	Flux	Focused beam size	Resolution	Technical Quality Metric
EPU105, EPU57	15-1550 eV		$\approx 10^{12}$ p/s	1µm(KB) 6 µm(Ellipsoid)	10^5 - 10^4	1

Names of Beamline Personnel and Fractional* FTEs in FY2016

ESM Operations		
ELIO	VESCOVO	0.17
ANDREW	WALTER	0.16
HUIJUAN	XU	0.07
SUSAN	MALDONADO	0.07
9 other staff members contributed effort		0.11
Total		0.58

*Note: 1.0 FTE based on 1760 hours of work. Some staff may log more hours annually

Funding source and fraction of funding for each source FY15-16

FY 2015: DOE – BES; 100%
FY 2016: DOE – BES; 100%
FY 2017: DOE – BES; 100%

Operating funds FY15-16 (K$)

Fiscal Year	Labor Costs	Contract Milestone Payments	Travel	Contract Labor, JT Appts & Shops	Maint/Svc Contracts	Materials & Purchasing	Total Cost
2015	n/a	n/a	n/a	n/a	n/a	n/a	n/a
2016	152K					10K	161K

Allocation Percentages

Fiscal Year**	Maintenance & Start up	General Users	Partner Users	Facility Staff
2015	n/a	n/a	n/a	n/a
2016	n/a	n/a	n/a	n/a
2017	90	9	0	1

** Partial year for 2017.

Number of unique beamline users each year

Fiscal Year**	General Users	Partner Users	Facility Staff	Total
2015	n/a	n/a	n/a	n/a
2016	0	0	4	4
2017	0	2	5	7

** Partial year for 2017.

Publications: (all publications used NSLS-II photons; numbers in parentheses indicates staff co-authorship)

Calendar Year**	Refereed	DOE High Profile	DOE High Impact	All Publications
2015	n/a	n/a	n/a	n/a
2016	n/a	n/a	n/a	n/a
2017	0	0	0	0

** Partial year for 2017.

Complete List of Publications for CY15-17

(includes publications that used NSLS-II photons, beamline R&D publications by staff, and staff research publications; red text indicates publications that used NSLS-II photons)

Refereed Journal Publications

- D Meyers, H Miao, A Walters, V Bisogni, R Springell, M d'Astuto, M Dantz, J Pelliciari, H Huang, et al., Doping Dependence of the Magnetic Excitations in La 2−x Sr x CuO 4, Phys. Rev. B: Condens. Matter, 95, 075139 (2017).
- C Carbone, P Moras, P Sheverdyaeva, D Pacile, M Papagno, L Ferrari, D Topwal, E Vescovo, G Bihlmayer, et al., Asymmetric Band Gaps in a Rashba Film System, Phys. Rev. B: Condens. Matter, 93, 125409 (2016).
- T Mentes, N Stojic, E Vescovo, J Ablett, M Nino, A Locatelli, Vacancy-mediated fcc/bcc Phase Separation in Fe1−xNix Ultrathin Films, Phys. Rev. B: Condens. Matter, 94, 085402 (2016).

22-IR-1 Frontier Synchrotron Infrared Spectroscopy (FIS)

Beamline Status

Construction

Overall Description

Scientific Scope

Infrared electronic and vibrational spectroscopy to understand the structure and behavior of materials under conditions of extreme pressures and temperatures as occur deep inside planets.

Description

Broad spectral range infrared beamline with endstations optimized for the study of materials at extreme temperatures and pressures. Includes diamond anvil cells, cryostats and laser heating cells.

Optical System

Mainly aluminum mirror relay optics

Experimental Apparatus

Commercial and custom microscopes for various diamond anvil cell configurations. Includes two FTIR spectrometers, Raman spectrometer, laser fluorescence spectrometer and microscope for pressure measurements. Sample cryostats for low T and CO₂ laser heating for high T

Computer System

PC workstations with Windows OS

Current Capabilities Available for Users (as of 1 May 2017)

N/A

Beamline Specifications

Source Type	Energy Range	Wavelength range	Flux	Focused beam size	Resolution	Technical Quality Metric

Dipole	0.1-4 eV					

Names of Beamline Personnel and Fractional* FTEs in FY2016

*Note: 1.0 FTE based on 1760 hours of work. Some staff may log more hours annually

Funding source and fraction of funding for each source FY15-16

FY 2015: DOE – BES; 100%
FY 2016: DOE – BES; 100%
FY 2017: DOE – BES; 100%

Operating funds FY15-16 (K$)

Fiscal Year	Labor Costs	Contract Milestone Payments	Travel	Contract Labor, JT Appts & Shops	Maint/Svc Contracts	Materials & Purchasing	Total Cost
2015	n/a	n/a	n/a	n/a	n/a	n/a	n/a
2016	n/a	n/a	n/a	n/a	n/a	n/a	n/a

Allocation Percentages

Fiscal Year**	Maintenance & Start up	General Users	Partner Users	Facility Staff
2015	n/a	n/a	n/a	n/a
2016	n/a	n/a	n/a	n/a
2017	0	50	40	10

** Partial year for 2017.

Number of unique beamline users each year

Fiscal Year**	General Users	Partner Users	Facility Staff	Total
2015	n/a	n/a	n/a	n/a
2016	n/a	n/a	n/a	n/a
2017	9	1	0	10

** Partial year for 2017.

Publications: (all publications used NSLS-II photons; numbers in parentheses indicates staff co-authorship)

Calendar Year**	Refereed	DOE High Profile	DOE High Impact	All Publications
2015	n/a	n/a	n/a	n/a
2016	n/a	n/a	n/a	n/a
2017	3 (0)	1 (0)	2 (0)	3 (0)

** Partial year for 2017.

Complete List of Publications for CY15-17

(includes publications that used NSLS-II photons, beamline R&D publications by staff, and staff research publications; red text indicates publications that used NSLS-II photons)

Refereed Journal Publications

- H Zhang, H Liu, K Wei, O Kurakevych, Y Le Godec, Z Liu, J Martin, M Guerrette, G Nolas, T Strobel, BC8 Silicon (Si-III) is a Narrow-Gap Semiconductor, Phys. Rev. Lett., 118, 146601 (2017).
- A Jaffe, Y Lin, W Mao, H Karunadasa, Pressure-Induced Metallization of the Halide Perovskite (CH3NH3)PbI3, J. Am. Chem. Soc., 139(12), 4330-4333 (2017).
- G Liu, L Kong, J Gong, W Yang, H Mao, Q Hu, Z Liu, R Schaller, D Zhang, T Xu, Pressure-Induced Bandgap Optimization in Lead-Based Perovskites with Prolonged Carrier Lifetime and Ambient Retainability, Adv. Func. Mater., 27(3), 1604208 (2017).

22-IR-2 Magnetospectroscopy, Ellipsometry and Time-Resolved Optical Spectroscopies (MET)

Beamline Status

Construction

Overall Description

Scientific Scope

Condensed matter physics spectroscopy: Studies of complex oxides exhibiting competing phases and emergent phenomena (e.g. multi-ferroics, topological insulators, high-Tc and conventional superconductors), and semiconductors for advanced energy applications. Also, optics and instrumentation development for synchrotron techniques.

Description

Beamline for infrared and optical spectroscopies, including Mueller-matrix ellipsometry and samples at low temperatures and high magnetic fields. Includes micro-sampling spectroscopy. Spectral range from millimeter waves to near UV.

Optical System

Aluminized mirror extraction and relay optics

Experimental Apparatus

Microscope with cryostat for small samples at low temperatures, 10T magnet cryostat, Mueller-matrix ellipsometer, synchronized Ti:sapphire laser (or similar) for photo-induced and pump-probe spectroscopies

Computer System

PC workstations with Windows OS

Current Capabilities Available for Users (as of 1 May 2017)

N/A

Beamline Specifications

Source Type	Energy Range	Wavelength range	Flux	Focused beam size	Resolution	Technical Quality Metric
Dipole	0.1-4 eV					

Names of Beamline Personnel and Fractional* FTEs in FY2016

*Note: 1.0 FTE based on 1760 hours of work. Some staff may log more hours annually

Funding source and fraction of funding for each source FY15-16

FY 2015: DOE – BES; 100%
FY 2016: DOE – BES; 100%
FY 2017: DOE – BES; 100%

Operating funds FY15-16 (K$)

Fiscal Year	Labor Costs	Contract Milestone Payments	Travel	Contract Labor, JT Appts & Shops	Maint/Svc Contracts	Materials & Purchasing	Total Cost
2015	n/a	n/a	n/a	n/a	n/a	n/a	n/a
2016	n/a	n/a	n/a	n/a	n/a	n/a	n/a

Allocation Percentages

Fiscal Year**	Maintenance & Start up	General Users	Partner Users	Facility Staff
2015	n/a	n/a	n/a	n/a
2016	n/a	n/a	n/a	n/a
2017	n/a	n/a	n/a	n/a

** Partial year for 2017.

Number of unique beamline users each year

Fiscal Year**	General Users	Partner Users	Facility Staff	Total
2015	n/a	n/a	n/a	n/a
2016	n/a	n/a	n/a	n/a
2017	n/a	n/a	n/a	n/a

** Partial year for 2017.

Publications: (all publications used NSLS-II photons; numbers in parentheses indicates staff co-authorship)

Calendar Year**	Refereed	DOE High Profile	DOE High Impact	All Publications
2015	n/a	n/a	n/a	n/a
2016	n/a	n/a	n/a	n/a
2017	n/a	n/a	n/a	n/a

** Partial year for 2017.

Complete List of Publications for CY15-17

(includes publications that used NSLS-II photons, beamline R&D publications by staff, and staff research publications; red text indicates publications that used NSLS-II photons)

Refereed Journal Publications

- T Huffman, C Hendriks, E Walter, J Yoon, H Ju, R Smith, G Carr, H Krakauer, M Qazibash, The Insulating Phases of Vanadium Dioxide are Mott-Hubbard Insulators, Phys. Rev. B: Condens. Matter, 95, 075125 (2017).
- B Ravel, G L Carr, C Hauzenberger, W Klysubun, X-ray and optical spectroscopic study of the coloration of red glass used in 19th century decorative mosaics at the Temple of the Emerald Buddha, J. Cultural Heritage, 16(3), 315-321 (2015).

23-ID-1 Coherent Soft X-ray Scattering (CSX-1)

Beamline Status

Operations

Overall Description

Scientific Scope

The Coherent Soft X-ray Scattering beamline (CSX-1) is a canted undulator beamline at sector 23-ID providing coherent soft x-ray scattering and imaging with world-leading high-coherent flux and detectors for probing correlated electronic textures and dynamics. Endstation instrumentation allows experiments using X-ray Photon Correlation Spectroscopy (XPCS), scanning diffraction microscopy, and coherent diffraction imaging.

Beamline Description

The CSX beamlines (CSX-1 and CSX-2) are served by two identical EPU49 sources. These EPUs serve the beamlines in three possible modes. 1) Both undulators in-line serving the CSX-1 branch to provide the highest coherent flux. 2) canted serving the CSX-2 branch to enable fast switching of two polarization states and 3) canted to allow simultaneous use of both branches.

Optical System

CSX-1 consists of a first (M1A) plane mirror, a VLS-PGM and a spherical bent mirror (M3A) resulting in a spot at the exit slit of ~20 um. The exit slit can be located ~1m upstream of the endstation to provide an ~200 um beam in the endstation or located in the endstation for coherent diffraction studies.

Experimental Apparatus

In-Vacuum Spectrometer with FastCCD (960x960 at 100Hz)

Computer System

Beamline components are controlled by EPICS. The user interface is through the Python and Control System Studio (CSS) clients. The user views the experimental system (sample and the surrounding environment) through CCD-coupled optical microscopes with Prosilica cameras. Linux Debian for running Workstations and IOCs.

Current Capabilities Available for Users (as of 1 May 2017)

- X-ray Scattering, coherent
- X-ray Scattering, magnetic
- X-ray Scattering, resonant

- Zone Plate based nano-diffraction
- Surface soft X-ray scattering

Beamline Specifications

Source Type	Energy Range	Wavelength range	Flux	Focused beam size	Resolution	Technical Quality Metric
EPU49	270 - 2000 eV	λ=6.2-45 Å	≈ 10^{13} p/s	20 µm (50 nm with zone plate)	5 x 10^{-3}	1

Names of Beamline Personnel and Fractional* FTEs in FY2016

CSX-1 Operations		
ANDI	BARBOUR	1.11
CLAUDIO	MAZZOLI	1.08
STUART	WILKINS	0.56
LARRY	FARERIA	0.34
DANIEL	BACESCU	0.19
WEN	HU	0.14
CHRISTOPHER	STELMACH	0.09
MARY	CARLUCCIDAYTON	0.09
SUSAN	MALDONADO	0.07
STEVE	OHARA	0.06
KAZIMIERZ	GOFRON	0.05
39 other staff members contributed effort		0.76
Total		4.54

*Note: 1.0 FTE based on 1760 hours of work. Some staff may log more hours annually

Funding source and fraction of funding for each source FY15-16

FY 2015: DOE – BES; 100%
FY 2016: DOE – BES; 100%
FY 2017: DOE – BES; 100%

Operating funds FY15-16 (K$)

Fiscal Year	Labor Costs	Contract Milestone Payments	Travel	Contract Labor, JT Appts & Shops	Maint/Svc Contracts	Materials & Purchasing	Total Cost
2015	1,280K	0	22K	36K	72K	282K	1,692K
2016	966K	0	1K	40K	62K	261K	1,330K

Allocation Percentages

Fiscal Year**	Maintenance & Start up	General Users	Partner Users	Facility Staff
2015	84.9	15.1	0	0
2016	39	49.1	7.4	4.5
2017	22	66	7	5

** Partial year for 2017.

Number of unique beamline users each year

Fiscal Year**	General Users	Partner Users	Facility Staff	Total
2015	11	0	5	16
2016	32	9	5	46
2017	23	7	7	37

** Partial year for 2017.

Publications: (all publications used NSLS-II photons; numbers in parentheses indicates staff co-authorship)

Calendar Year**	Refereed	DOE High Profile	DOE High Impact	All Publications
2015	1 (1)	0 (0)	0 (0)	1 (1)
2016	1 (1)	1 (1)	1 (1)	2 (2)
2017	0 (0)	0 (0)	0 (0)	0 (0)

** Partial year for 2017.

Complete List of Publications for CY15-17

(includes publications that used NSLS-II photons, beamline R&D publications by staff, and staff research publications; red text indicates publications that used NSLS-II photons)

Refereed Journal Publications

- X Chen, V Thampy, C Mazzoli, A Barbour, H Miao, G Gu, Y Cao, Remarkable Stability of Charge Density Wave Order in La1.875Ba0.125CuO4, Phys. Rev. Lett., 117, 167001 (2016).
- J Zhong, J Kestell, I Waluyo, S Wilkins, C Mazzoli, A Barbour, K Kaznatcheev, M Shete, M Tsapatsis, J Boscoboinik, Oxidation and Reduction under Cover: Chemistry at the Confined Space between Ultrathin Nanoporous Silicates and Ru(0001), J. Phys. Chem. C, 120, 8240-8245 (2016). [111991]
- D Porter, M Senn, K Khalyavin, A Cortese, N Waterfield-Price, P Radaelli, P Manuel, H zur-Loye, C Mazzoli, A Bombardi, Magnetostriction-driven Ground-state Stabilization in 2H Perovskites, Phys. Rev. B: Condens. Matter, 94, 134404 (2016).
- C Zhu, R Harder, A Diaz, V Komanicky, A Barbour, R Xu, X Huang, Y Liu, M Pierce, et al., Ptychographic X-ray Imaging of Surfaces on Crystal Truncation Rod, Appl. Phys. Lett., 106(10), 101604 (2015). [107614]

Refereed Conference Proceedings

- H Fernandes, C Kitegi, D Harder, D Hidas, J Rank, M Musardo, P Cappadoro, T Tanabe, Coherent Soft x-ray Epu Vacuum Chamber Thermal Analysis for Synchrotron Radiation Protection, MEDSI, Vol 1, p. 1-3, sponsored by ALBA Light Source (2016).
- F Willeke, Commissioning of NSLS-II, Proceedings of IPAC2015, p. 11-16, sponsored by PAC2015 (2015).

23-ID-2 Soft X-ray Spectroscopy and Polarization (CSX-2)

Beamline Status

Operations

Overall Description

Scientific Scope

The Coherent Soft X-ray Scattering and Spectroscopy beamline (CSX-2) is a canted undulator beamline at sector 23-ID for in situ soft x-ray spectroscopic studies of surface processes in heterogeneous catalysis and other energy systems. Ambient pressure photoelectron spectroscopy (AP-PES), available for general user experiments, allows XPS measurements to be performed at elevated pressures (up to 5 Torr). This bridges the pressure gap problem in catalysis between ideal surface science experiments and industrial catalytic processes. X-ray absorption spectroscopy (XAS) is available for science commissioning on UHV-compatible powder and thin film samples using TEY and PFY detection modes. In situ reactor cells are under development.

Beamline Description

The CSX beamlines (CSX-1 and CSX-2) are served by two identical EPU49 sources. These EPUs serve the beamlines in three possible modes. 1) Both undulators in-line serving the CSX-1 branch to provide the highest coherent flux. 2) canted serving the CSX-2 branch to enable fast switching of two polarization states and 3) canted to allow simultaneous use of both branches.

Optical System

Variable line spacing - plane grating monochromator (VLS-PGM).

Experimental Apparatus

1. Ambient pressure photoelectron spectroscopy (AP-PES) endstation with SPECS PHOIBOS 150 NAP electron analyzer. Operating pressure up to 5 Torr. Sample heating is available up to 900 C in UHV and ~500 C in higher pressures (depending on the type of gas). Sputter ion gun is available for sample cleaning. A 4-pocket e-beam evaporator is available for metal deposition.

Available standard gases: Ar, H_2, O_2, CO, CO_2, CH_4, C_2H_6, C_2H_4, H_2O, methanol, ethanol. Other gases or liquid vapors must be arranged in advance with beamline staff. Liquids with boiling point above 100 C are not allowed.

2. In situ and operando X-ray absorption spectroscopy (IO-XAS) endstation with total electron yield and Vortex SDD partial fluorescence yield detector. Currently, only UHV-compatible solid samples (powders, thin films, crystals) are allowed.

Computer System

Beamline components are controlled by EPICS. The user interface is through the Python and Control System Studio (CSS) clients. The user views the experimental system (sample and the surrounding environment) through CCD-coupled optical microscopes with Prosilica cameras. Linux Debian for running Workstations and IOCs.

Current Capabilities Available for Users (as of 1 May 2017)

- Ambient Pressure X-ray Photoelectron Spectroscopy
- Soft X-ray absorption spectroscopy of UHV compatible powder samples in partial fluorescence yield and total electron yield detection modes
- Multimodality 3D imaging with higher resolutions.

Beamline Specifications

Source Type	Energy Range	Wavelength range	Flux	Focused beam size	Resolution	Technical Quality Metric
EPU49	270 - 2000 eV	λ=6.2-45 Å	$5x10^{12}$ p/s	16 x 40 µm2	$1x10^{-4}$	1

Names of Beamline Personnel and Fractional* FTEs in FY2016

CSX-2 Operations		
IRADWIKANARI	WALUYO	1.10
ADRIAN	HUNT	0.50
PETER	CAPPADORO	0.18
LARRY	FARERIA	0.10
KAZIMIERZ	GOFRON	0.09
MARY	CARLUCCIDAYTON	0.09
JAMES	RANK	0.07
CHRISTOPHER	STELMACH	0.07
GUILLERMO	APARICIO	0.07
SUSAN	MALDONADO	0.07
HUSTON	FERNANDES	0.07
KONSTANTINE	KAZNATCHEEV	0.06
CHRISTOPHER	STEBBINS	0.05
CHARLES	KITEGI	0.05
60 other staff members contributed effort		1.1
Total		3.67

*Note: 1.0 FTE based on 1760 hours of work. Some staff may log more hours annually

Funding source and fraction of funding for each source FY15-16

FY 2015: DOE – BES; 100%
FY 2016: DOE – BES; 100%
FY 2017: DOE – BES; 100%

Operating funds FY15-16 (K$)

Fiscal Year	Labor Costs	Contract Milestone Payments	Travel	Contract Labor, JT Appts & Shops	Maint/Svc Contracts	Materials & Purchasing	Total Cost
2015	532K	0	0	72K	66K	202K	872K
2016	750K	0	4K	19K	15K	239K	1,026K

Allocation Percentages

Fiscal Year**	Maintenance & Start up	General Users	Partner Users	Facility Staff
2015	100	0	0	0
2016	39	49.1	7.4	4.5
2017	27	5	16	7

** Partial year for 2017.

Number of unique beamline users each year

Fiscal Year**	General Users	Partner Users	Facility Staff	Total
2015	0	1	6	7
2016	40	8	7	55
2017	36	12	6	54

** Partial year for 2017.

Publications: (all publications used NSLS-II photons; numbers in parentheses indicates staff co-authorship)

Calendar Year**	Refereed	DOE High Profile	DOE High Impact	All Publications
2015	0 (0)	0 (0)	0 (0)	0 (0)
2016	2 (2)	0 (0)	0 (0)	2 (2)
2017	0 (0)	0 (0)	0 (0)	0 (0)

** Partial year for 2017.

Complete List of Publications for CY15-17

(includes publications that used NSLS-II photons, beamline R&D publications by staff, and staff research publications; red text indicates publications that used NSLS-II photons)

Refereed Journal Publications

- J Kestell, J Zhong, M Shete, I Waluyo, J Sadowski, D Stacchiola, M Tsapatsis, J Boscoboinik, Studying Two-dimensional Zeolites with the Tools of Surface Science: MFI Nanosheets on Au(111), Catal. Today, 280(2), 238-288 (2016).
- J Zhong, J Kestell, I Waluyo, S Wilkins, C Mazzoli, A Barbour, K Kaznatcheev, M Shete, M Tsapatsis, J Boscoboinik, Oxidation and Reduction under Cover: Chemistry at the Confined Space between Ultrathin Nanoporous Silicates and Ru(0001), J. Phys. Chem. C, 120, 8240-8245 (2016).
- M Wang, J Zhong, J Kestell, I Waluyo, D Stacchiola, J Boscoboinik, D Lu, Energy Level Shifts at the Silica/Ru(0001) Heterojunction Driven by Surface and Interface Dipoles, Top Catal (2016). doi:10.1007/s11244-016-0704-x

Other Publications (books, theses, etc)

- R Palomino, E Stavitski, I Waluyo, Y Chen-Wiegart, M Abeykoon, J Sadowski, J Rodriguez, A Frenkel, S Senanayake, New In-Situ and Operando Facilities for Catalysis Science at NSLS-II: The Deployment of Real-Time, Chemical, and Structure-Sensitive X-ray Probes, Synch. Rad. News, 30(2), 30-37 (2017).

28-ID-1 Total Scattering Beamline (PDF)

Beamline Status

Construction

Overall Description

Scientific Scope

X-ray Powder Diffraction-1 (XPD-1) is the dedicated atomic Pair Distribution Function (PDF) beamline at the NSLS-II. XPD-1 enables studies of nanoscale fluctuations and hidden broken symmetry phases in next generation complex materials.

Beamline Description

The X-ray Powder Diffraction (XPD) beamline at NSLS-II consists of two branch lines, the high- resolution powder diffraction beamline, XPD-2 and the dedicated Atomic Pair Distribution Function (PDF) beamline, XPD-1. The damping wiggler, DW100 delivers a large energy band-pass white X-ray beam into the First Optical Enclosure (FOE) of the beamline. The horizontally focusing Side Bounce Monochromator (SBM) at XPD-1 receives the part of the white beam that is transmitted through the first crystal of the XPD-2 Double Laue Monochromator (DLM). The SBM is used to select the X-ray photon energy at XPD-1. The vertical focusing of the beam is achieved by using a long bent mirror mounted further downstream in the FOE. XPD-1 offers rapid data acquisition rates (30 frames/s) and high flux required for in-situ operando studies. A wide variety of sample environments including (80 – 500) K Liquid nitrogen cryostream, (5-500) K cryostat, (0-5) T superconducting magnet and gas flow-cells are available at the beamline. Beamline is equipped with an automatic capillary sample alignment system. XPD-1 offers real-time data processing and analysis capabilities with a suite of user-friendly robust software.

Optical System

Laue Side Bounce Monochromator, Vertically Focusing Mirror, Automatic energy calibration system, Laser alignment system.

Experimental Apparatus

2 Area detectors, (80 - 500) K cryostream, (5 - 500) K cryostat, 5 T Superconducting magnet, gas handling system, IR furnace, Automatic sample alignment system.

Computer System

Debian Linux Servers, xPDF Suite, VisTrails, QXRD, Fit2D, EPICS, Python.

Current Capabilities Available for Users (as of 1 May 2017)

N/A

Beamline Specifications

Source Type	Energy Range	Wavelength range	Flux	Focused beam size	Resolution	Technical Quality Metric
DW100	39 - 117 keV (4 discrete energies)	0.32 - 0.10 Å	≈ 2-6 x 10^{13} p/s	1.5 mm (Ho) x 0.024 mm (Ve)	~ $2x10^{-2}$ - $4x10^{-3}$	1

Names of Beamline Personnel and Fractional* FTEs in FY2016

*Note: 1.0 FTE based on 1760 hours of work. Some staff may log more hours annually

Funding source and fraction of funding for each source FY15-16

FY 2015: DOE – BES; 100%
FY 2016: DOE – BES; 100%
FY 2017: DOE – BES; 100%

Operating funds FY15-16 (K$)

Fiscal Year	Labor Costs	Contract Milestone Payments	Travel	Contract Labor, JT Appts & Shops	Maint/Svc Contracts	Materials & Purchasing	Total Cost
2015	n/a	n/a	n/a	n/a	n/a	n/a	n/a
2016	n/a	n/a	n/a	n/a	n/a	n/a	n/a

Allocation Percentages

Fiscal Year**	Maintenance & Start up	General Users	Partner Users	Facility Staff
2015	n/a	n/a	n/a	n/a
2016	n/a	n/a	n/a	n/a
2017	n/a	n/a	n/a	n/a

** Partial year for 2017.

Number of unique beamline users each year

Fiscal Year**	General Users	Partner Users	Facility Staff	Total
2015	n/a	n/a	n/a	n/a
2016	n/a	n/a	n/a	n/a
2017	n/a	n/a	n/a	n/a

** Partial year for 2017.

Publications: (all publications used NSLS-II photons; numbers in parentheses indicates staff co-authorship)

Calendar Year**	Refereed	DOE High Profile	DOE High Impact	All Publications
2015	n/a	n/a	n/a	n/a
2016	n/a	n/a	n/a	n/a
2017	n/a	n/a	n/a	n/a

** Partial year for 2017.

Complete List of Publications for CY15-17

(includes publications that used NSLS-II photons, beamline R&D publications by staff, and staff research publications; red text indicates publications that used NSLS-II photons)

Refereed Journal Publications

- R Palomino, E Stavitski, I Waluyo, Y Chen-Wiegart, M Abeykoon, J Sadowski, J Rodriguez, A Frenkel, S Senanayake, New In-Situ and Operando Facilities for Catalysis Science at NSLS-II: The Deployment of Real-Time, Chemical, and Structure-Sensitive X-ray Probes, Synch. Rad. News, 30(2), 30-37 (2017).
- A Kudielka, S Bette, R Dinnebier, M Abeykoon, C Pietonka, B Harbrecht, Variability of Composition and Structural Disorder of Nanocrystalline CoOOH Materials, J. Mater. Chem. C, 5, 2899 (2017).
- L Li, X Deng, Z Wang, Y Liu, M Abeykoon, E Dooryhee, A Tomic, Y Huang, J Warren, et al., Superconducting Order from Disorder in 2H-TaSe2-xSx, 2, 11 (2017).
- M Retuerto, S Skiadopoulou, M Li, A Abakumov, M Croft, A Ignatov, T Sarkar, B Abbett, M Abeykoon, et al., Pb2MnTeO6 Double Perovskite: An Antipolar Anti-ferromagnet, Inorg. Chem., 55(9), 4320-4329 (2016).
- H Ryu, M Abeykoon, E Bozin, Y Matsumoto, S Nakatsuji, C Petrovic, Multiband Electronic Transport in Alpha-Yb(1-x)Sr(x)AIB(4) [x=0, 0.19(3)] Single Crystals , J. Phys.: Condens. Matter, 28(42), 425602 (2016).
- H Ryu, M Abeykoon, K Wang, H Lei, N Lazarevic, J Warren, E Bozin, Z Popovic, C Petrovic, Insulating and Metallic Spin Glass in Ni-doped KxFe2−ySe2 Single Crystals, Phys. Rev. B: Condens. Matter, 91(18), 184503 (2015).

- M Abeykoon, H Hu, L Wu, Y Zhu, S Billinge, Calibration and Data Collection Protocols for Reliable Lattice Parameter Values in Electron Pair Distribution Function Studies, J. Appl. Cryst., 48(1), 244-251 (2015). [107933]
- H Ryu, M Abeykoon, K Wang, H Lei, N Lazarevic, J Warren, E Bozin, Z Popovic, C Petrovic, Insulating and Metallic Spin Glass in Ni-doped KxFe2−ySe2 Single Crystals, Phys. Rev. B: Condens. Matter, 91, 184503 (2015). [108122]

28-ID-2 X-ray Powder Diffractions (XPD)

Beamline Status

Operations

Overall Description

Scientific Scope

The X-ray Powder Diffraction (XPD) beamline serves a very broad and diverse user community ranging from physics, chemistry, and materials science to earth science, environmental science and engineering science. XPD operates with photon beams whose energy is fully tunable between 40 keV and 70 keV, with a nominal beam size of 0.6×0.2 mm^2. Hard X-rays provide the opportunity to probe high-Z or bulk samples, buried interfaces, and through sample cells and devices. The core mission of XPD is to observe materials under conditions that are far from equilibrium, non ambient or non static, i.e., as a function of a process parameter like T, P, pH, reactive gases, electric or magnetic field.

Major focus themes of XPD are: 1) in situ synthesis (e.g., high temperature solid state growth, colloidal nanoparticles from solution, flash sintering of ceramics/oxide materials, nucleation & growth of MOFs, and microwave-assisted synthesis) and 2) in situ structure evolution (e.g., catalysis, oxidation reduction reactions using gases, hydrogenation reactions, gas adsorption and separation, and cycling of energy-storage devices). Theory and experiment can be integrated in a closed loop in exploratory syntheses, where theory can identify theoretical desired materials that are thermodynamically stable, and in situ XRD synthesis could then be used to pinpoint the feasible synthetic routes. This new approach has great potential to accelerate materials discovery.

Beamline Description

XPD is configured for near-field (higher Q coverage) and far-field (higher Q resolution, i.e., better peak separation) 2D diffraction. For this purpose, endstation C hosts two large-area detectors that consist of flat scintillator panels (16”×16” active area, CsI coated, 0.2mm pixels). They can be quickly interchanged at any time in the course of a reaction or a process. This dual detector arrangement is ideal for total scattering measurements that provide both long-range and short-range order information on any material in exactly the same environment and set-up. The crystalline fraction of the sample is examined by Rietveld refinements using the XRD data and the model is subsequently imported as a .CIF (Crystallographic Information File) for use in the modeling of the short-range order based on the PDF data.

Thanks to the high energy of the photon beam, a significant portion of the diffraction space can be captured in one shot by the large-area detectors (i.e., without scanning). Therefore XPD is well suited for sub-minute data collection times, ideal for time-dependent measurements of transformations or transient processes. A robotic sample changer is available for high-throughput measurements. XPD also offers a large variety of sample environments (commercial, user-

custom or in-house systems) that include: furnaces, cryostats, flow cells, etc. Together, these make XPD a world-class facility in the field of in situ and operando structural science.

XPD will offer the option of a high-resolution configuration (for structure solving and line profile analysis) by trading its 1D and 2D detectors for a unique system composed of 8 channels fitted with analyzer Laue crystals. It will use two distinct detector units developed in house, that are angle-scanned simultaneously and collect the sample-diffracted signal with and without the analyzer crystals. One unit is an array of photomultiplier tubes associated with GYSO scintillator crystals. The second unit is an array of 8 × 8 CdZnTe chips.

A second endstation (hutch D - not in use yet) of XPD will accommodate more elaborate/complex setups: large pressure cells, diffraction-tomography, non-routine reaction chambers, combined spectrometry, gas handling, user-custom devices, etc. Beam spot will be reduced to 20microns using an assembly of focusing mirrors. Hutch D will also be used for those measurements that require long lead-time preparation, e.g., a gas rig or a spectrometer. Alternatively the beam can be sent intermittently into hutch D to enable short and repetitive measurements at regular intervals over a long period of time i.e., corrosion studies, slow growth processes, charging and discharging of batteries, degradation of cathodes and anodes in fuel cell research, environmental effects on solar cell materials.

Techniques: powder diffraction, total scattering (PDF), small/medium angle scattering (SAXS, MAXS), tomography (CT). Opportunities for in-situ and in-operando structural science (variety of sample environments, functional materials in working conditions or in operating devices).

Optical System

Laue-Laue monochromator for beam energy selection with a 0.1% energy bandwidth and sagittal focusing 2) Coated mirror for vertical focusing/collimation 3) Channel-cut monochromator with a narrower energy bandwidth for high resolution powder diffraction.

Experimental Apparatus

XPD operates essentially in transmission mode, either in capillary or flat plate geometries.

Equipment of endstation C includes: 1) a 3-circles diffractometer; 2) two Flat Panel detectors for 2D diffraction; 3) a Pixel Array Detector; 4) a multi-channel analyzer system; 5) an extensive suite of sample environments (commercial and user-custom) for in situ diffraction.

Available sample cells include: lamp furnace (RT- 2000C); Linkam flat plate furnace (RT-1500C); hot air blower (RT - 1000C); gas flow reactors and flexible coil heater for capillaries; reaction cell (400C, 1500psi); microwave heater; cryostream (80K - 800K); He cryostat (10K - RT); multi-purpose cell (oxidative/corrosive gases, laser heating up to 1100C, 3D stress by a 4-point bending system, vertical and axial loads up to 20 lbs)

Computer System

Beamline components are controlled by EPICS. Delta Tau Geobrick LV is the standard controller for stepper motors. The user interface is implemented using Python and Control System Studio (CSS) clients operating under Linux Debian workstations with CPU and GPU clusters, and offering local and centralized data storage.

Software:

Ophyd: a python-based ("spec-like") command line interface for scanning

Bluesky: a library for experiment control and collection of scientific data and metadata (http://nsls-ii.github.io/bluesky/)

XpdAcq (http://xpdacq.github.io/) is a python package that aids data collection at the XPD beamlime. It is built on top of and augments the NSLS-II data acquisition Python package Bluesky.

Current Capabilities Available for Users (as of 1 May 2017)

- Nominal beam size = 0.60 x 0.20 mm^2
- Energy range = 40-70keV (tunable)
- X-ray Powder Diffraction using a large area (2k x 2k pixels) detector (200micron pixel), distance to sample can be varied
- X-ray Pair Distribution Function measurements using another large area (2k x 2k pixels) detector (200 micron pixel) – Qmax is 27Angstrom-1
- Small Angle X-ray Scattering for detecting particles and precipitates smaller than 100nm
- Flat plate or capillary, transmission (recommended) and reflection geometries
- High-throughput, capillary measurements using the robotic arm
- Available sample cells include: lamp furnace (RT- 2000°C); Linkam flat plate furnace (RT- 1500°C); hot air blower (RT - 1000°C); gas flow reactors and flexible coil heater for capillaries; reaction cell (400°C, 1500psi); cryostream (80K - 800K); He cryostat (10K - RT); multi-purpose cell (oxidative/corrosive gases, 3D stress, vertical and axial loads up to 20 lbs)
- Modulation Enhanced Diffraction using electric field
- Testing of a Germanium microstrip detector
- Testing of a 2Θ-driven pixel array, photon counting CdTe detector (active surface is: 10 x 15mm^2)
- Diamond Anvil High Pressure Cell (Max ~40 GPa)
- High Pressure Gas/liquid flow cell (max 150 bar)
- Reactor for microwave-assisted synthesis

Beamline Specifications

Source Type	Energy Range	Wavelength range	Flux	Focused beam size	Resolution	Technical Quality Metric
DW100	40-70 KeV	0.17-0.31	≈ 8 x 10^{12} p/s	500 µm Ho x 50 µm Ve	10^{-3} - 2x10^{-4}	1

Names of Beamline Personnel and Fractional* FTEs in FY2016

XPD Operations		
SANJIT	GHOSE	1.03
ERIC	DOORYHEE	0.94
JOHN	TRUNK	0.73
AM	ABEYKOON	0.72
JIANMING	BAI	0.71
HANFEI	YAN	0.24
MARY	CARLUCCIDAYTON	0.09
SUSAN	MALDONADO	0.07
EDWIN	HAAS	0.06
QINGFU	TANG	0.05
40 other staff members contributed effort		0.90
Total		5.52

*Note: 1.0 FTE based on 1760 hours of work. Some staff may log more hours annually

Funding source and fraction of funding for each source FY15-16

FY 2015: DOE – BES; 100%
FY 2016: DOE – BES; 100%
FY 2017: DOE – BES; 100%

Operating funds FY15-16 (K$)

Fiscal Year	Labor Costs	Contract Milestone Payments	Travel	Contract Labor, JT Appts & Shops	Maint/Svc Contracts	Materials & Purchasing	Total Cost
2015	1,517K	42K	14K	174K	12K	140K	1,900K
2016	1,450K	42K	33K	44K	22K	50K	1,640K

Allocation Percentages

Fiscal Year**	Maintenance & Start up	General Users	Partner Users	Facility Staff
2015	49.7	17	3.3	0
2016	42.3	51.7	3.8	2.2
2017	32	56	8	4

** Partial year for 2017.

Number of unique beamline users each year

Fiscal Year**	General Users	Partner Users	Facility Staff	Total
2015	33	0	4	37
2016	94	11	4	109
2017	90	3	6	99

** Partial year for 2017.

Publications: (all publications used NSLS-II photons; numbers in parentheses indicates staff co-authorship)

Calendar Year**	Refereed	DOE High Profile	DOE High Impact	All Publications
2015	3 (3)	0 (0)	0 (0)	5 (5)
2016	18 (6)	0 (0)	1 (1)	21 (9)
2017	3 (2)	0 (0)	1 (1)	4 (2)

** Partial year for 2017.

Complete List of Publications for CY15-17

(includes publications that used NSLS-II photons, beamline R&D publications by staff, and staff research publications; red text indicates publications that used NSLS-II photons)

Refereed Journal Publications

- N Simos, Z Zhong, E Dooryhee, S Ghose, S Gill, F Camino, I Savkhyidiz, E Akdogan, Neutron Irradiation and High Temperature Effects on Amorphous Fe-based Nano-coatings on Steel e A Macroscopic Assessment, J. Nucl. Mat., 489, 164-179 (2017).
- L Li, X Deng, Z Wang, Y Liu, M Abeykoon, E Dooryhee, A Tomic, Y Huang, J Warren, et al., Superconducting Order from Disorder in 2H-TaSe2-xSx, NPJ Quantum Materials, 2, 11 (2017).
- A Plonka, Q Wang, W Gordon, A Balboa, D Troya, W Guo, C Sharp, S Senanayake, J Morris, et al., In Situ Probes of Capture and Decomposition of Chemical Warfare Agent Simulants by Zr-Based Metal Organic Frameworks, J. Am. Chem. Soc., 139(2), 599-602 (2017).
- F Bertolotti, L Protesescu, M Kovalenko, S Yakunin, A Cervellino, S Billinge, M Terban, J Pedersen, N Masciocchi, A Guagliardi, Coherent Nanotwins and Dynamic Disorder in Cesium Lead Halide Perovskite Nanocrystals, ACS Nano, 11 (4), 3819–3831 (2017).
- X Ma, K An, J Bai, H Chen, NaAlTi3O8, A Novel Anode Material for Sodium Ion Battery, Sci. Rep., 7, 162 (2017).
- L Wangoh, Y Huang, R Jezorek, A Kehoe, G Watson, F Omenya, N Quackenbush, N Chernova, M Whittingham, L Piper, Correlating Lithium Hydroxyl Accumulation with Capacity Retention in V2O5 aerogel cathodes, ACS Appl. Mater. Interfaces, 8(18), 11532-11538 (2016).
- B Frandsen, L Liu, S Cheung, Z Guguchia, R Khasanov, E Morenzoni, T Munsie, A Hallas, M Wilson, et al. , Volume-wise Destruction of the Antiferromagnetic Mott Insulating State Through Quantum Tuning, Nat. Commun., 7, 12519 (2016).
- B Anasori, C Shi, E Ju Moon, Y Xie, C Voigt, P Kent, S May, S Billinge, M Barsoum, Y Gogotsi, Control of Electronic Properties of 2D Carbides (MXenes) by Manipulating their Transition Metal Layers, Nanoscale Horiz., 1(3), 227-234 (2016).
- A Beecher, O Semonin, J Skelton, J Frost, M Terban, H Zhai, A Alatas, J Owen, A Walsh, S Billinge, Direct Observation of Dynamic Symmetry Breaking above Room Temperature in Methylammonium Lead Iodide Perovskite, ACS Energy Lett., 1(4), 880-887 (2016).
- X Yang, Y Zhou, J Yue, E Hu, H Li, L Gu, K Nam, S Bak, X Yu, J Liu, High-Rate Charging Induced Intermediate Phases and Structural Changes of Layer-Structured Cathode for Lithium-Ion Batteries, Adv. Energy Mater., 6(21), 1600597 (2016).
- J Zhao, W Zhang, A Huq, S Misture, B Zhang, S Guo, L Wu, Y Zhu, Z Chen, et al., In Situ Probing and Synthetic Control of Cationic Ordering in Ni-Rich Layered Oxide Cathodes, Adv. Energy Mater., 7(3), 1601266 (2016).
- C Cama, C Pelliccione, A Brady, J Li, E Stach, J Wang, E Takeuchi, K Takeuchi, A Marschilok, Redox Chemistry of a Binary Transition Metal Oxide (AB2O4): a Study of the Cu2+/Cu0 and Fe3+/Fe0 Interconversions Observed Upon Lithiation in a CuFe2O4 battery using X-ray Absorption Spectroscopy, Phys. Chem. Chem. Phys., 18, 16930-16940 (2016).
- B Frandsen, Z Gong, M Terban, S Banerjee, B Chen, C Jin, M Feygenson, Y Uemura, S Billinge, Local Atomic and Magnetic Structure of Dilute Magnetic Semiconductor (Ba,K)(Zn,Mn)2As2, Phys. Rev. B: Condens. Matter, 94, 094102 (2016).
- A Wang, I Zaliznyak, W Ren, L Wu, D Graf, V Garlea, J Warren, E Bozin, Y Zhu, C Petrovic, Magnetotransport Study of Dirac Fermions in YbMnBi2 Antiferromagnet , Phys. Rev. B: Condens. Matter, 94(16), 165161 (2016).
- E Hu, Y Lyu, H Xin, J Liu, L Han, S Bak, J Bai, Y Yu, H Li, X Yang, Explore the Effects of Microstructural Defects on Voltage Fade of Li- and Mn-Rich Cathodes, Nano Lett., 16, 5999-6007 (2016).

- J Liu, L Yin, L Wu, J Bai, S Bak, X Yu, Y Zhu, X Yang, P Khalifah, Quantification of Honeycomb Number-Type Stacking Faults: Application to Na3Ni2BiO6 Cathodes for Na-Ion Batteries, Inorg. Chem., 55(17), 8478-8492 (2016).
- M Elbakhshwan, S Gill, A Motta, R Weidner, T Anderson, L Ecker, Sample Environment for in situ Synchrotron Corrosion Studies of Materials in Extreme Environments, Rev. Sci. Instrum., 87(10), 105122 (2016).
- J Liu, Y Amit, Y Li, A Plonka, S Ghose, L Zhang, E Sach, U Banin, A Frenkel, Reversed Nanoscale Kirkendall Effect in Au–InAs Hybrid Nanoparticles, Chem. Mater., 28, 8032-8043 (2016).
- D Hudry, A Abeykoon, E Dooryhee, D Nykypanchuk, J Dickerson, Probing the Crystal Structure and Formation Mechanism of Lanthanide-Doped Upconverting Nanocrystals, Chem. Mater., 28(23), 8752-8763 (2016).
- R Zhang, T Abtew, N Quackenbush, L Wangoh, M Huie, A Brady, D Bock, H Efstathiadis, M Whittingham, et al., Electrode Reaction Mechanism of Ag2VO2PO4 Cathode, Chem. Mater., 28(10), 3428-3434 (2016).
- J Xu, F Lin, D Nordlund, E Crumlin, F Wang, J Bai, M Doeff, W Tong, Elucidation of the Surface Characteristics and Electrochemistry of High-performance LiNiO2, Chem. Commun., 52, 4239-4242 (2016).
- J Arinez-Soriano, J Jorge Albalad, A Carne-Sanchez, C Bonnet, F Busque, J Lorenzo, J Juanhuix, M Terban, I Imaz, et al., pH-Responsive Relaxometric Behaviour of Coordination Polymer Nanoparticles Made of a Gadolinium Macrocyclic Chelate, Chem. Eur. J., 22(37), 13162-13170 (2016).
- A Colli, K Attenkofer, B Raghothamachar, M Dudley, Synchrotron X-Ray Topography for Encapsulation Stress/Strain and Crack Detection in Crystalline Silicon Modules, IEEE J. Photovoltaics, 6(5), 1387-1389 (2016).
- R Caliandro, T Sibillano, B Belviso, R Scarfiello, J Hanson, E Dooryhee, M Manca, P Cozzoli, C Giannini, Static and Dynamical Structural Investigations of Metal-Oxide Nanocrystals by Powder X-ray Diffraction: Colloidal Tungsten Oxide as a Case Study, ChemPhysChem, 17(5), 699-709 (2016). [112193]
- X Yang, E Hu, Y Lyu, E Dooryhee, X Yu, H Li, H Xin, Important Roles of Crystallinity in Voltage Fade of Li- and Mn-Rich Cathodes Exemplified By Li2Ru0.5Mn0.5O3 Studies, 18th International Meeting on LIthium Batteries, sponsored by IMLB (2016).
- K Takeuchi, L Wu, F Xu, A Brady, J Durham, J Huang, Q Meng, M Kaltak, E Dooryhee, et al., One Dimensional Manganese Oxides As Cathode Materials in Li-Ion Batteries: The Impact of Physicochemical Properties on Electrochemical Performance, 18th International Meeting on LIthium Batteries, sponsored by IMLB (2016).
- J Sinsheimer, N Bouet, S Ghose, E Dooryhee, R Conley, Fabrication and Testing of a Newly Designed Slit System for Depth-resolved X-ray Diffraction Measurements, J. Synch. Rad., 23, 1296-1304 (2016). [112332]
- E Rus, G Moon, J Bai, D Steingart, C Erdonmez, Electrochemical Behavior of Electrolytic Manganese Dioxide in Aqueous KOH and LiOH Solutions: A Comparative Study, J. Electrochem. Soc., 163(3), A356-363 (2016).
- H Xu, X Guo, J Bai, Thermal Behavior of Polyhalite: a High-temperature Synchrotron XRD Study, Phys. Chem. Miner., 44, 125-135 (2016).
- Y Zhou, J Yue, E Hu, H Li, L Gu, K Nam, S Bak, X Yu, J Bai, et al., High-Rate Charging Induced Intermediate Phases and Structural Changes of Layer-Structured Cathode for Lithium-Ion Batteries , Adv. Energy Mater., 6(21), 1600597 (2016).
- X Hong, L Ehm, Z Zhong, S Ghose, T Duffy, D Weidner, High-energy X-ray Focusing and Applications to Air Distribution Function Investigation of Pt and Au Nanoparticles at High Pressures, Sci. Rep., 6, 21434 (2016).

- N Simos, M Elbakhshwan, Z Zhong, S Ghose, I Savkliyildiz, High-temperature Annealing of Proton Irradiated Beryllium - a Dilatometry-based Study, J. Nucl. Mat., 477(15), 1-17 (2016).
- M Elbakhshwan, K McDonald, S Ghose, Z Zhong, N Simos, X-ray Diffraction Studies of 145 MeV Proton-irradiated AlBeMet 162, 8, 8-17 (2016).
- N Simos, Z Zhong, S Ghose, H Kirk, L Trung, K McDonald, Z Kotsina, P Nocera, R Assmann, et al., Radiation Damage and Thermal Shock Response of Carbon-fiber-reinforced Materials to Intense High-energy Proton Beams, Phys. Rev. Accel. Beams, 19, 111002 (2016).
- L Wu, F Xu, Y Zhu, A Brady, J Huang, J Durham, E Dooryhee, A Marschilok, E Takeuchi, K Takeuchi, Structural Defects of Silver Hollandite, AgxMn8Oy, Nanorods: Dramatic Impact on Electrochemistry, ACS Nano, 9(8), 8430-8439 (2015).
- K Wang, A Wang, A Tomic, L Wang, A Abeykoon, E Dooryhee, S Billinge, C Petrovic, Enhanced Thermoelectric Power and Electronic Correlations in RuSe2, APL Mater., 3(4), 041513 (2015).
- K Jensen, A Blichfeld, S Bauers, S Wood, E Dooryhee, D Johnson, B Iversen, S Billinge, Demonstration of Thin Film Pair Distribution Function Analysis (tfPDF) for the Study of Local Structure in Amorphous and Crystalline Thin Films, IUCrJ, 2, 481-489 (2015).
- D Sprouster, J Sinsheimer, E Dooryhee, S Ghose, P Wells, T Stan, N Almirall, G Odette, L Ecker, Structural Characterization of Nanoscale Intermetallic Precipitates in Highly Neutron Irradiated Reactor Pressure Vessel Steels, Scripta Mater., 113(1), 18-22 (2015).
- F Xin, X Wang, J Bai, W Wen, H Tian, C Wang, W Han, A Lithiation/Delithiation Mechanism of Monodispersed MSn5 (M=Fe, Co and FeCo) Nanospheres, J. Mater. Chem. A, 3, 7170-7178 (2015).
- T Nguyen-Phan, S Luo, D Vovchok, J LIorca, J Graciani, J Fernandez Sanz, S Sallis, W Xu, J Bai, et al., Visible Light-Driven H2 Production over Highly Dispersed Ruthenia on Rutile TiO2 Nanorods, ACS Catal., 6(1), 407-417 (2015).
- J Krogstad, Y Gao, J Bai, J Wang, D Lipkin, C Levi, In Situ Diffraction Study of the High-Temperature Decomposition of t′-Zirconia, J. Am. Ceram. Soc., 98(1), 247-254 (2015). [107490]
- J Bai, J Hong, H Chen, J Graetz, F Wang, Solvothermal Synthesis of LiMn1–xFexPO4 Cathode Materials: A Study of Reaction Mechanisms by Time-Resolved in Situ Synchrotron X-ray Diffraction, J. Phys. Chem. C, 119(5), 2266-2276 (2015). [107764]
- J Patete, M Scofield, V Volkov, C Koenigsmann, Y Zhang, A Marschilok, X Wang, J Bai, J Han, et al., Ambient Synthesis, Characterization, and Electrochemical Activity of LiFePO4 Nanomaterials Derived from Iron Phosphate Intermediates, Nano Res., 8(8), 2573-2594 (2015).
- L Wang, J Bai, P Gao, X Wang, J Looney, F Wang, Structure Tracking Aided Design and Synthesis of Li3V2 PO4)3 Nanocrystals as High-Power Cathodes for Lithium Ion Batteries, Chem. Mater., 27(16), 5712-5718 (2015).
- X Chen, A Plonka, D Banerjee, R Krishna, H Shaef, S Ghose, P Thallapally, J Parise, Direct Observation of Xe an Kr adsroption in a Xe-selective Microporous Metal-Organic Framework, J. Am. Chem. Soc., 137(22), 7007-7010 (2015).

Refereed Conference Proceedings

- A Howansky, A Lubinsky, S Ghose, K Suzuki, W Zhao, Direct Measurement of Lubberts effect in CsI:Tl scintillators using single x-ray photon imaging, SPIE Medical Imaging 2017, Vol 10132, sponsored by SPIE (2017).
- M Okuniewski, L Ecker, M Elbakshwan, D Sprouster, D Velazquez, R Siebert, D Lee, J Terry, Y Sohn, et al., High Energy X-ray Applications for the Characterization of Metallic Uranium Alloys, Transactions of the American Nuclear Society,, Vol 114, sponsored by NSUF (2016).

Other Publications (books, theses, etc)

- R Palomino, E Stavitski, I Waluyo, Y Chen-Wiegart, M Abeykoon, J Sadowski, J Rodriguez, A Frenkel, S Senanayake, New In-Situ and Operando Facilities for Catalysis Science at NSLS-II: The Deployment of Real-Time, Chemical, and Structure-Sensitive X-ray Probes, Synch. Rad. News, 30(2), 30-37 (2017).
- L Ecker, D Sprouster, G Odette, N Almirall, T Stan, P Wells, T Novakowski, First Science at NSLS-II: Experimental Results and Data Analysis, BNL prepared for U.S. Department of Energy Nuclear Energy Enabling Technology (2017).
- L Ecker, D Sprouster, M Elbakshwan, S Ghose, E Doooryhee, G Odette, N Almirall, T Stan, P Wells, Automated Synchrotron Studies on Irradiated Materials: Experimental Results, BNL prepared for U.S. Department of Energy Nuclear Energy Enabling Technology (2016).
- L Ecker, D Sprouster, R Weidner, S Ghose, E Doooryhee, J Sinsheimer, M Elbakshwan, S Yoo, G Odette, et al., Final Technical Report on Automated Synchrotron X-ray Diffraction of Irradiated Materials, BNL prepared for U.S. Department of Energy Nuclear Energy Enabling Technology (2016).
- D Sprouster, A Hansen, E Dooryhee, L Ecker, R Pokharel, H Reiche, A Raftery, D Byler, K McClellan, Advanced Fuels Campaign 2016 Accomplishments: In Situ Synchrotron characterization of the Field Assisted Sintering of UO2 at the National Synchrotron Light Source –II, Idaho National Laboratory prepared for U.S. Department of Energy Nuclear Energy (2016).
- L Ecker, D Sprouster, M Elbakshwan, J Sinsheimer, S Ghose, E Dooryhee, G Odette, N Almirall, T Stan, et al., Second Annual Progress Report: Automated Synchrotron X-ray Diffraction of Irradiated Materials, BNL prepared for U.S. Department of Energy Nuclear Energy Enabling Technology (2015).
- L Ecker, D Sprouster, M Elbakshwan, J Sinsheimer, S Ghose, E Dooryhee, G Odette, N Almirall, T Stan, P Wells, First Science Experiment at NSLS-II: Development and Commissioning of Infrastructure, BNL prepared for U.S. Department of Energy Nuclear Energy Enabling Technology (2015).