Beamline & Experimental Operations

Paul Zschack, Director, Photon Science Division, NSLS-II

Triennial Operations Peer Review

June 20th 2017

“Beamline Operations” Outline

- Mission statement
- Current status
- Budget FY15-17
- Evolution of organization since 2015
- Future Plans
- Summary

Photon Science Division Mission & Strategy

- Photon Science Division operates state-of-the-art beamlines for a broad, scientifically diverse user community
- Photon Science Division staff lead new beamline development efforts (with user community), develop new experimental instruments & methods, collaborate with users, and produce high impact science using NSLS-II and other facilities
- Photon Science Division staff perform R&D for new developments in x-ray synchrotron science

We recruit excellent scientific and technical staff to address these objectives and prioritize support consistent with our strategic plan. We strive to 1) increase the number of NSLS-II users; 2) increase high impact science productivity; and 3) exploit the unique capabilities of the NSLS-II source by building and operating world-leading experimental facilities.

CURRENT STATUS

Beamlines: Current Status

General User Operations

CSX-1, CSX-2, XPD, HXN, SRX

IXS, CHX, LIX, AMX, FMX, ISS, XFP

Science Commissioning

TES, CMS, ISR

Technical Commissioning

ESM, SMI, NYX, SIX

Completion* in FY17

BMM, QAS, XFM, FXI

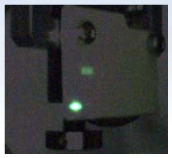
Completion* in FY18

PDF, FIS, MET, SST-1, SST-2

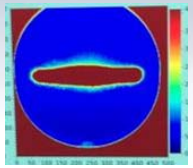
14 BES beamlines now taking beam
20 BES-operated beamlines in FY2018
28 total beamlines operating in FY2018

* Completion defined as having completed IRR

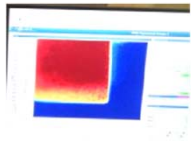
First Light Images: FY16



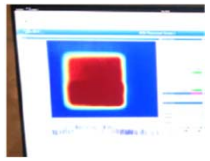
LIX Nov 16, 2015



ISS April 5, 2016

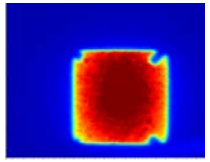


FMX March 8, 2016

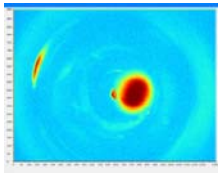


AMX March 8, 2016

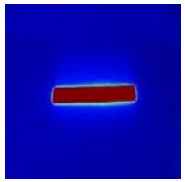
XFP July 11, 2016



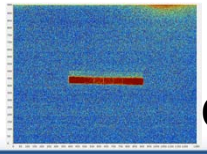
ISR July 11, 2016



ESM July 25, 2016

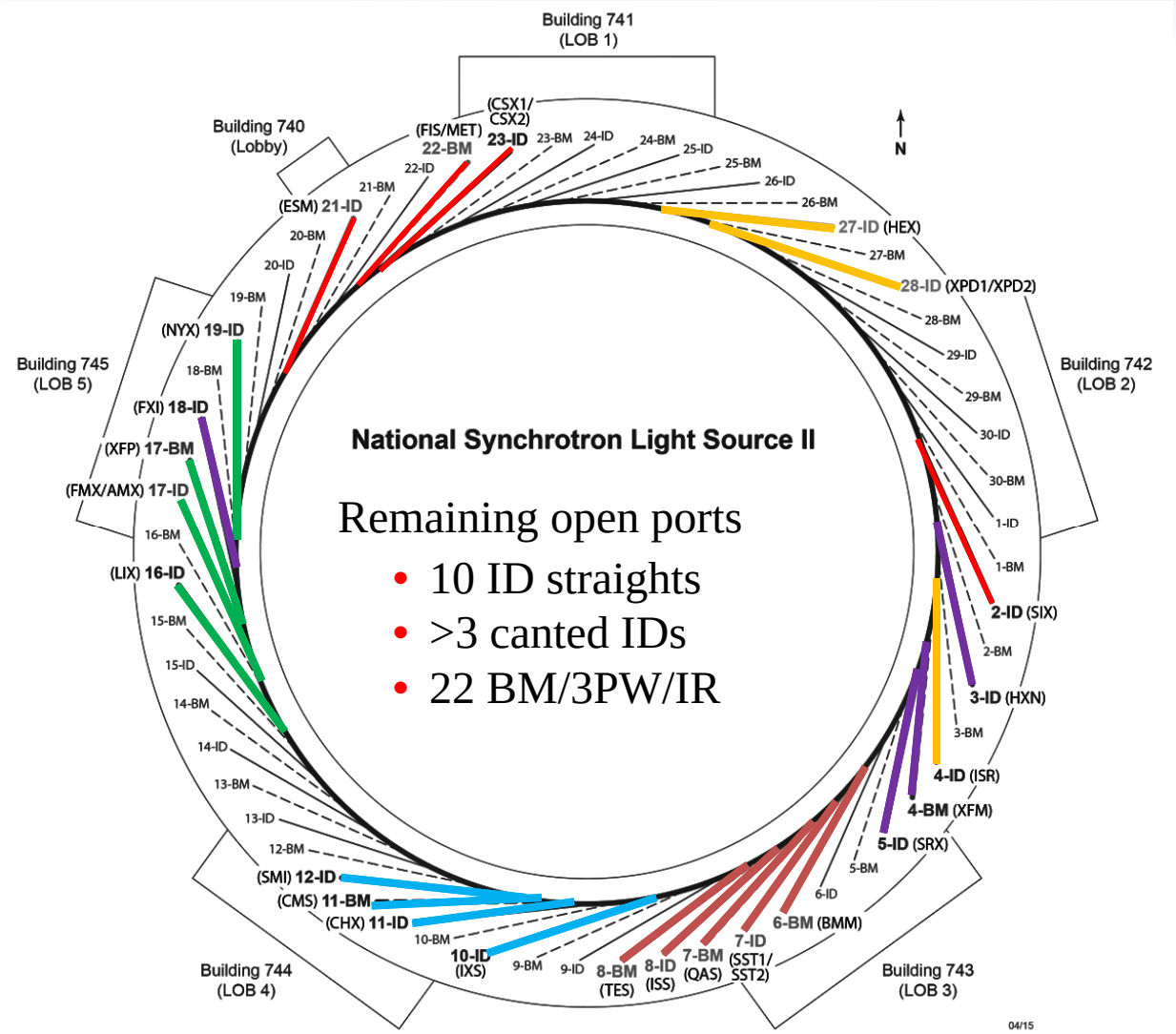


TES Aug 19, 2016



CMS Aug 29, 2016

NSLS-II Beamline Portfolio



Soft X-Ray Scattering & Spectroscopy

23-ID-1: Coherent Soft X-ray Scat (2015)
23-ID-2:Coherent Soft X-ray Spectr & Pol (2015/2016)
21-ID: Photoemission-Microscopy Facility (2017)
2-ID: Soft Inelastic X-ray Scattering (2017)
22-BM: Magneto, Ellipso, High Pressure IR (2018)

Complex Scattering

10-ID: Inelastic X-ray Scattering (2015)
11-ID: Coherent Hard X-ray Scattering (2015)
11-BM: Complex Materials Scattering (2016)
12-ID: Soft Matter Interfaces (2017)

Diffraction & In Situ Scattering

28-ID-1: X-ray Powder Diffraction (2015)
28-ID-2: X-ray Powder Diffraction (2017)
4-ID: In-Situ & Resonant X-Ray Studies (2017)
27-ID: High Energy X-ray Diffraction (2022)

Hard X-Ray Spectroscopy

8-ID: Inner Shell Spectroscopy (2017)
7-BM: Quick X-ray Absorption and Scattering (2016)
8-BM: Tender X-ray Absorption Spectroscopy (2017)
7-ID-1: Spectroscopy Soft and Tender (2017)
7-ID-2: Spectroscopy Soft and Tender (2017)
6-BM: Beamline for Mater. Measurements (2017)

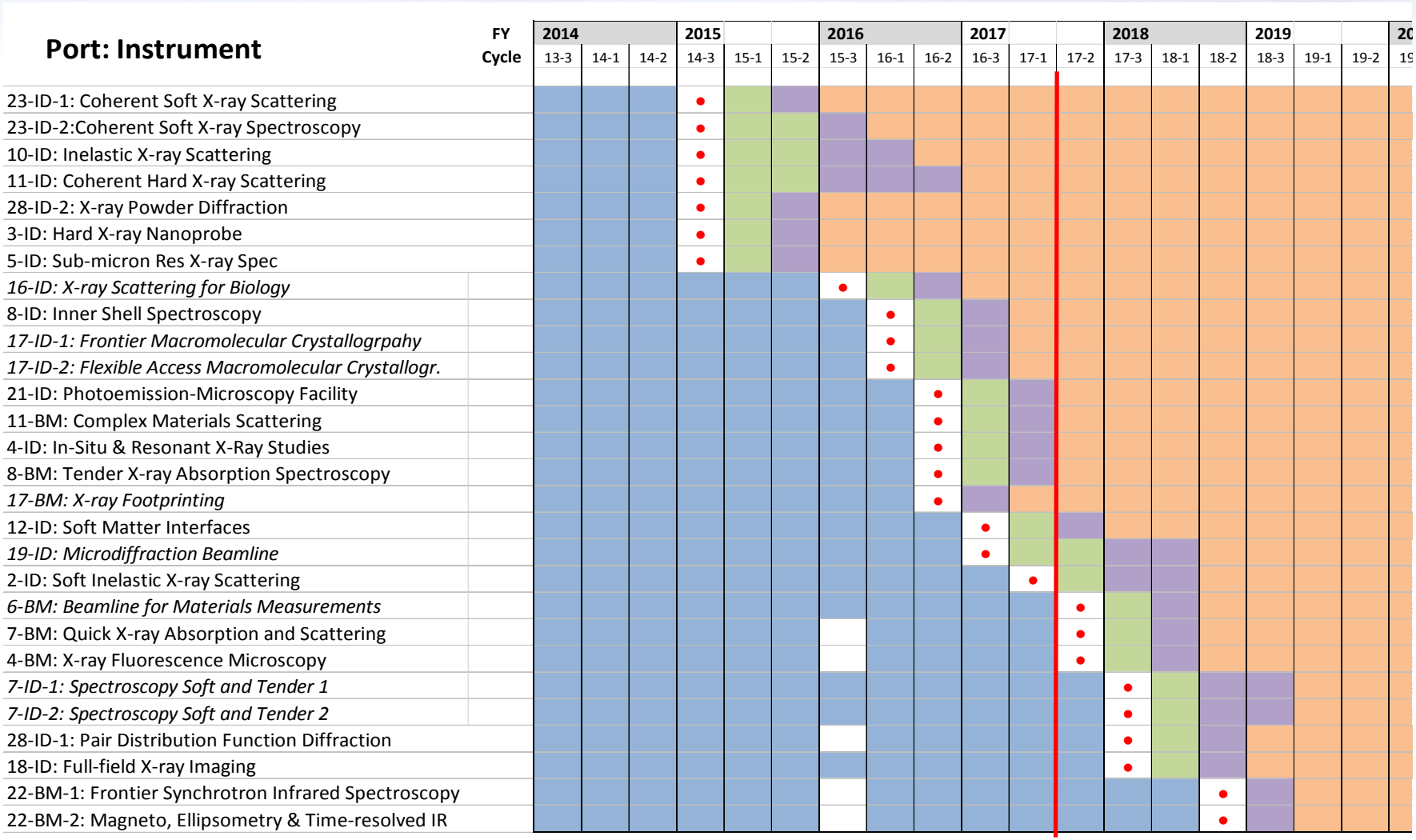
Imaging & Microscopy

3-ID: Hard X-ray Nanoprobe (2015)
5-ID: Sub-micron Res X-ray Spec (2015)
4-BM: X-ray Fluorescence Microscopy (2017)
18-ID: Full-field X-ray Imaging (2018)

Structural Biology

17-ID-1: Frontier Macromolecular Cryst (2016)
17-ID-2: Flexible Access Macromolecular Cryst (2016)
16-ID: X-ray Scattering for Biology (2016)
17-BM: X-ray Footprinting (2016)
19-ID: Microdiffraction Beamline (2017)

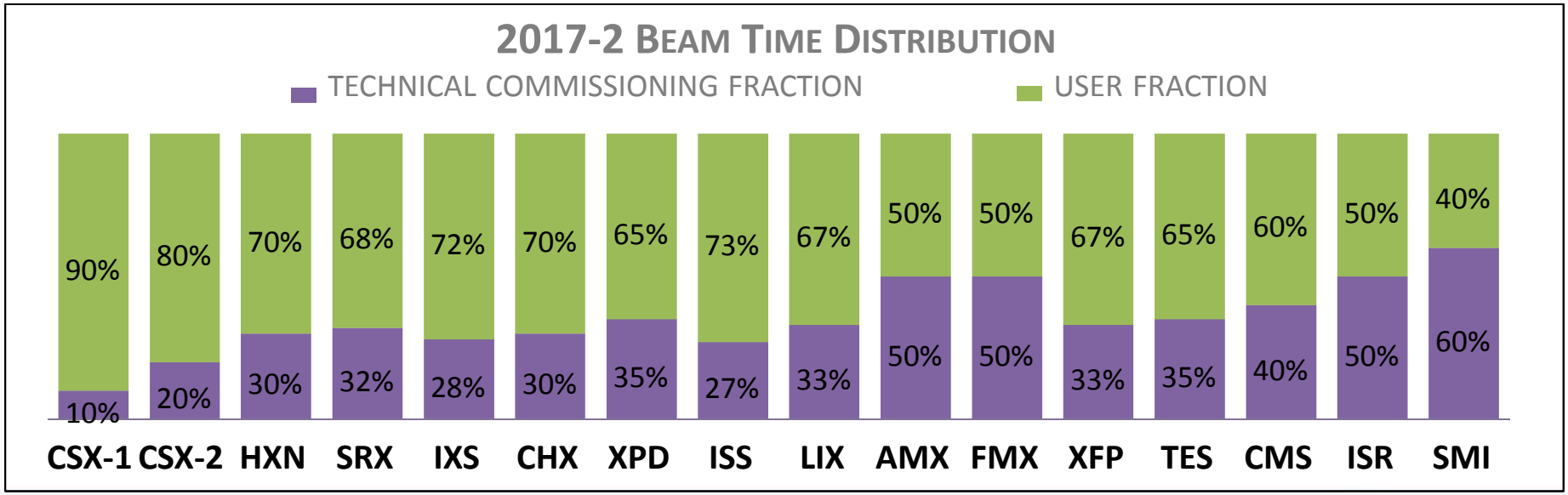
NSLS-II Beamline Buildout



- First light date

Phased Commissioning Approach

- Most beamlines have more than one capability or technique
- Scientific capabilities most likely to produce early science results are commissioned first based on scientific priorities determined through interactions with user community
- User science program begins once a scientific capability or technique is commissioned, and additional commissioning will alternate with previously commissioned science capabilities
- This "Phased Commissioning" approach allows a thorough technical commissioning of all planned science capabilities **and** will achieve early, high impact scientific productivity



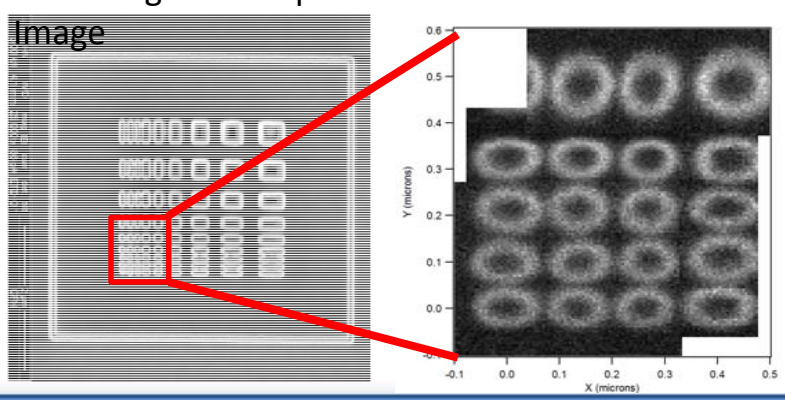
Beamline Complexity

- NSLS-II beamlines are designed to exploit the NSLS-II source and have very demanding performance specifications
- Complex motion controls and feed back systems are deployed to keep photon beams appropriately positioned. For example, HXN uses 2 fast feedback systems (100 Hz), 4 slow feedback systems (10 Hz), and has 18 nanopositioning feedback systems on the Zone Plate and MLL focusing systems
- Delivering and operating world-leading beamlines requires considerable complexity

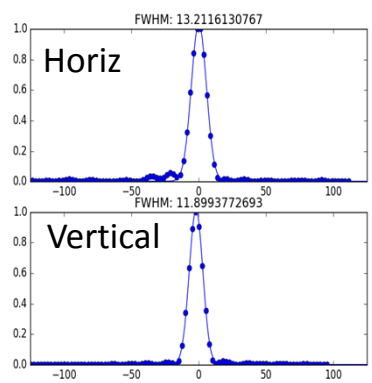
Beamline	# motors	# iocs/servers	PVs	Estimated Data rate (TB/day)	# diagnostic modules, bpms	# feedback systems	# BL vacuum sections	# major optical components	# Endstations
HXN	~300	107	~90000	11.8	7	2+4+18	14	5	2

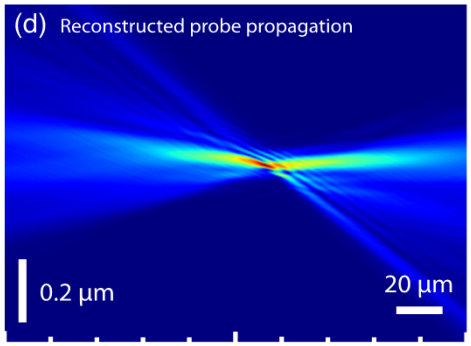
SEM image of test pattern

Pt Fluorescence



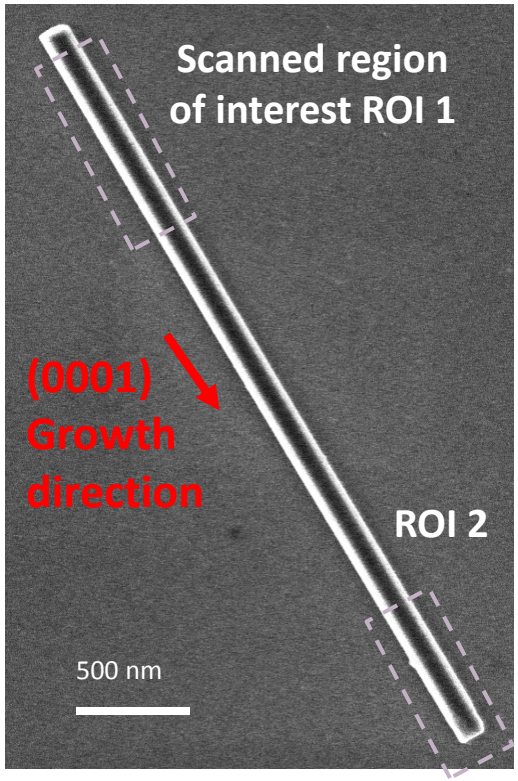
~ 11 x 13 nm resolution





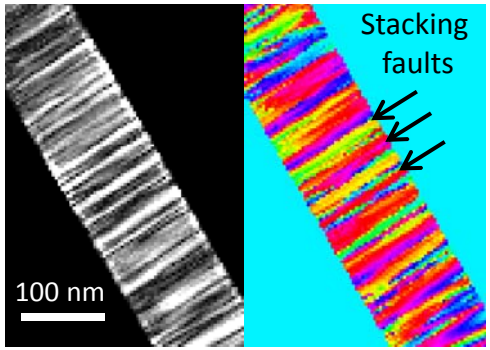
Imaging Strain and Stacking Faults (SF)

$In_{1-x}Ga_xAs$ nanowires (x=0.14)
Catalyst-free, site-selective growth by MBE on Si(111)

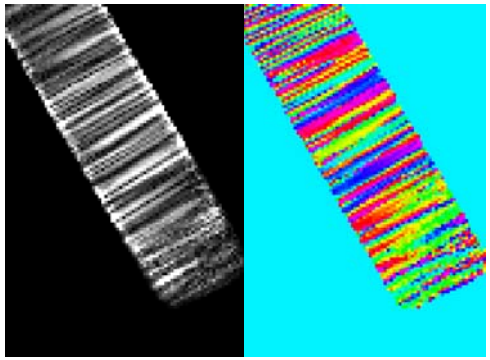


(20-20): sensitive to SF

ROI 1

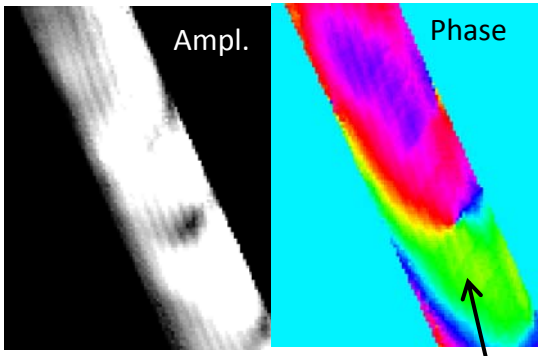


ROI 2



(2-1-12) insensitive to SF

ROI 1



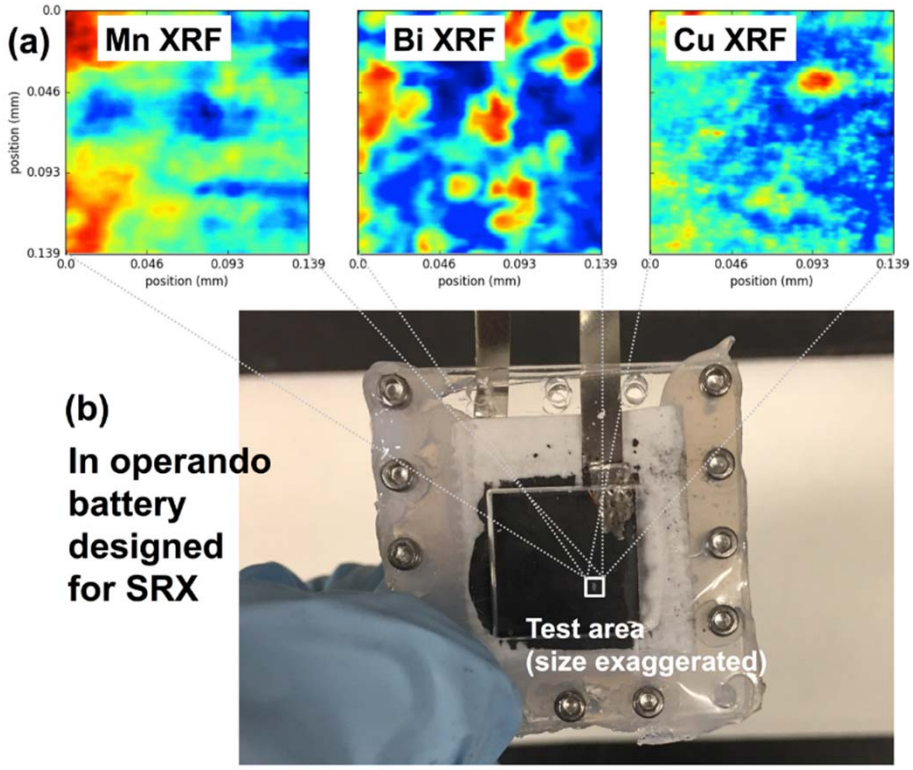
Slowly varying strain field

- Imaging reveals variation in stacking fault density along growth direction.
- Strain found to be largely uniform over ~100nm scale.
- ~ 8 nm resolution based on signal.
- Sampling resolution of 3.6nm/pixel.
- 2 min/image using fly-scan.

Hruszkewycz, Holt, Stephenson – ANL
Hill, Lauhon – Northwestern U.
Huang, Yan, Chu, Nazaretski – NSLS-II
Treu, Morkötter, Koblmueller – TU Munich

Copper Insertion into Bi-Modified MnO_2 Cathodes

- Batteries for grid applications for solar or wind power must be low cost, have high cycle life and energy density, be safe & reliable, and be composed of easily acquired, inexpensive materials.
- Aqueous Zn-MnO_2 with Cu and Bi additives may provide a safe alternative to Li-ion batteries
- High resolution elemental tracking reveals the slow incorporation of Cu into a MnO_2 cathode, increasing conductivity and allowing it to achieve high cycle life.



G. Yadav, et.al., *Nature Communications* **8**:14424, 2017

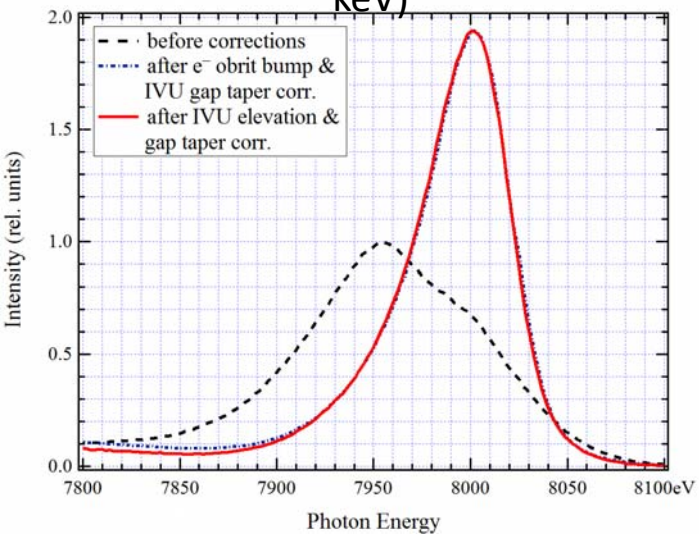
- Operando X-ray fluorescence microscopy at SRX showed that Cu begins highly coordinated with Bi spatially, and shifts to a correlation with Mn during initial cycling.
- Micro-XANES showed that a zero-valence Cu is produced at the bottom of discharge, inserting into the MnOOH structure and improving conductivity.
- Reversible formation of Cu^{2+}-intercalated Bi-δ-MnO_2 is confirmed by XANES analysis of an electrode that was cycled 60 times

(a) X-ray fluorescence microprobe imaging of Mn, Bi, and Cu in the battery cathode. (b) Photography of the test battery designed for the SRX beamline at NSLS-II.

Beamline Commissioning

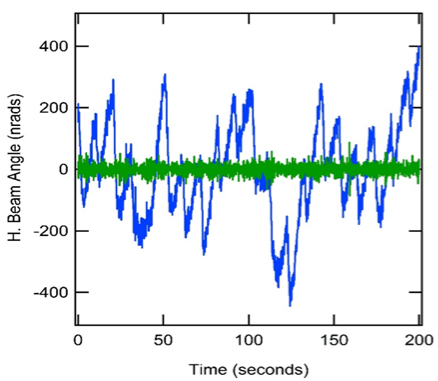
- Considerable progress toward bringing initial NSLS-II beamlines to full design performance
- Systematic approach for optimizing ID performance underway
- Slew scanning complex motions together with undulator has been challenging
- Beamlines are very sensitive to external influences; Stability taskforce created to address stability issues

IVU21 - 1.5 m at SRX BL
(harm. #5 at ~6.8 mm gap, ~8.0 keV)

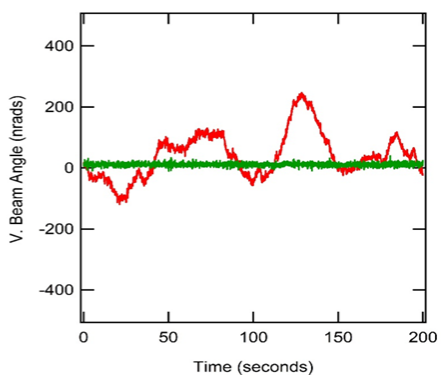


Spectral performance was fully restored by introducing +300 µm change in elevation and -35 µm change in taper.

Horizontal

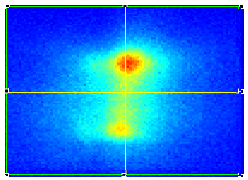


Vertical



Improvement due to feedback implementation at HXN

Beam at FMX (1 x 1.5 µm)



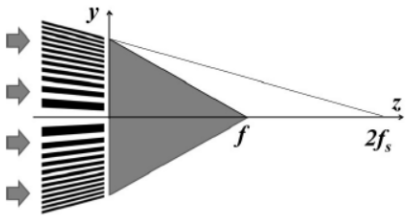
People walking on hutch roof, climbing stairs

Photon Science Division R&D

MLL fabrication

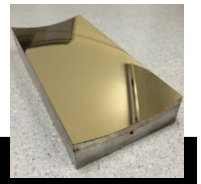
Advances in wedged MLL growth to produce smaller focus with increased efficiency.

Fabricated 25 μm thick wedged MLL with ~10nm zone placement error (designed for 15keV, f~2.5mm and focus size targeted of 8nm). Wedged MLL have been measured at APS – preliminary estimate 35% efficient. Fabricated wedged MLL with new materials (VSi_2/Si)

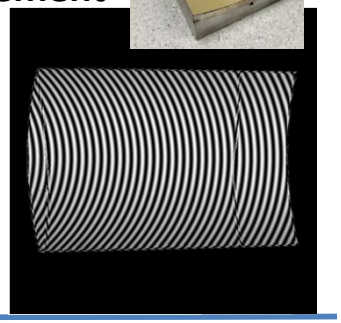


Phase Measuring Deflectometry for Mirror Metrology

Method eliminates the slope-height ambiguity in mirror figure measurement



Fringe patterns reflected by a mirror from an LCD display are captured by a camera, which will be used as feature points for an optimization with a mirror surface model to minimize their discrepancy in ray tracing



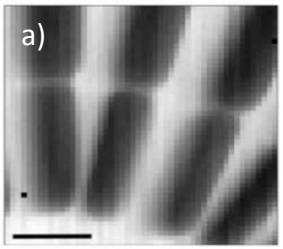
Detector developments

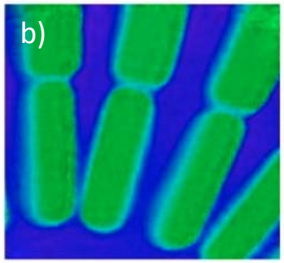
The VIPIC (*Vertically Integrated Photon Imaging Chip)* under development with a full-scale (i.e. 1 megapixel) version planned.

Detector optimized for XPCS experiments is essential for accessing micro-second time regimes and is ideally suited for a high-coherence X-ray scattering beamline, CHX.

Nano-positioning

A bonded MLL pair with 17×38 nm^2 point focus significantly simplifies the optical alignment complexity, thus greatly extending its applications in both scanning and full-field X-ray microscopies.

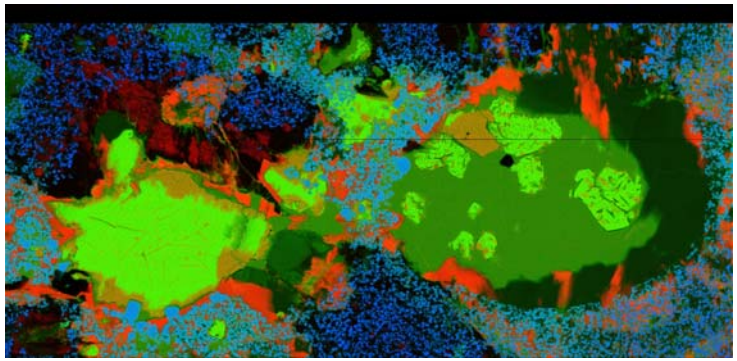




(a) STXM image and (b) ptychography reconstruction of the star test pattern. The scale bar is 250 nm, and the reconstructed image resolution is 13x13 nm^2

Photon Science Division R&D Priorities

Priorities set by importance to NSLS-II beamlines and resulting high impact science productivity



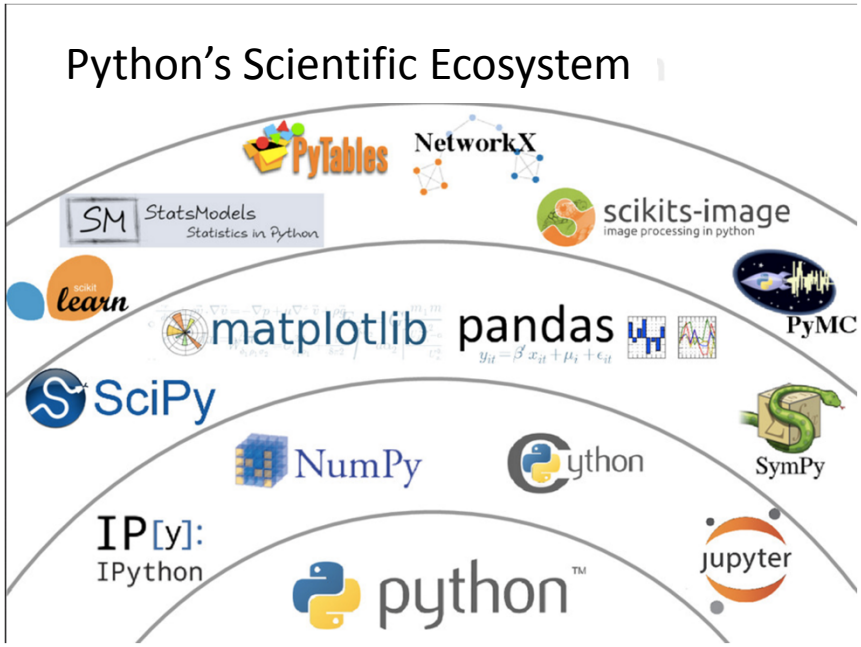
MAIA installed at SRX: image shows Rb-Fe-Cr in natural rock from Siberia. 7M-pixel image with pixel size 1μmx1μm measured in 3 hrs

- Nano-positioning developments
- Optical Metrology (characterization)
- Detector R&D
- Simulations
- MLL developments toward sub-5nm probe
- Kinoform R&D*
- At-wavelength metrology*
- Ion beam figuring of mirrors*

* Externally supported activities

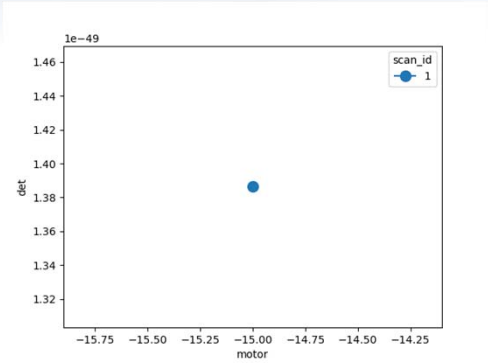
Data Acquisition Management Analysis Approach

- Exploit Scientific Python ecosystem & leverage python developments elsewhere
- Use standard tools where they exist, e.g. CAMERA (ptychography, Xi-Cam); APS (e.g. Tomopy, LMFit, etc..)
- Wherever possible, deploy existing software that has wide community acceptance
  - Users will be already familiar with them.
  - If authors are willing we can help provide hooks into our data architecture.
- Enable access to larger computational resources (HPC) such as NERSC or the BNL Institutional Cluster for users that require them.
- Hack-a-thons with BES user facilities
- Collaborate with other facilities that install and use the NSLS-II codes
- Hold workshops and tutorials to train staff and users

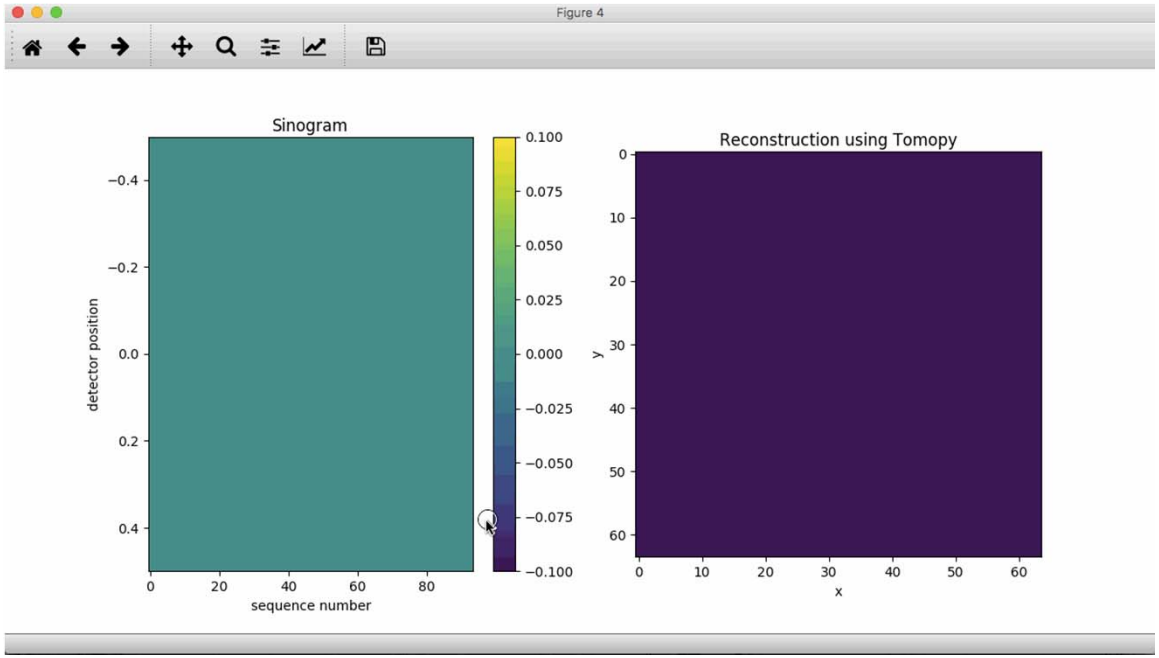


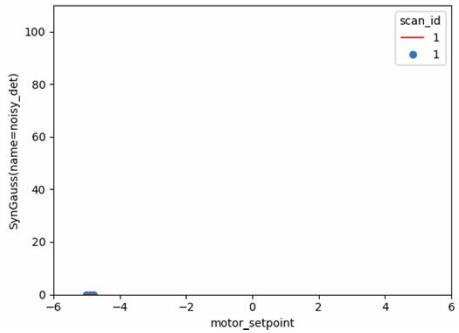
Data Acquisition Management Analysis Features

- New, modern software environment capable of handling the requirements of NSLS-II beamlines
- Supports compute and data storage local to the beamline, in the NSLS-II central computer room, and to BNL data center (or elsewhere)
- Will enable users to access and analyze their data during experiments and afterwards



Adaptive logic where each step is determined adaptively in response to local slope.





A Gaussian is fit to a stream of measured data using the Python library *lmfit (developed at APS)*.

A stream of images from a detector is reconstructed into a volume using *tomopy*.

Notable recognition

- “Novel hard x-ray scanning microscope with Multilayer Laue Lens nanofocusing optics” named a 2016 R&D 100 Award Winner (HXN team with ANL)
- “Binary Pseudo-Random Calibration Tool”, a test surface for determining imaging and profiling instrument modulation transfer functions. 2015 R&D 100 Award winner (Nathalie Bouet & Peter Takas with LBL and ANL)
- HXN won Microscopy Today Innovation Award 2016
- Innovate Long Island honors Innovators of the Year (Yong Chu & Evgeny Nazaretski)
- Google Open Source Peer Bonus winner (Tom Caswell)
- BNL 2015 Engineering Award winner (Evgeny Nazaretski)

R&D 100 2016 R&D 100 Awards

Microscopy TODAY 2016 Innovation Award

INNOVATELI INSIDE THE NEW ECONOMY 2017

Google Open Source matplotlib

BUDGET OVERVIEW

“Beamline Operations” Budget and Spending

	FY2015		FY2016		FY2017	
	FTEs	Burdened Costs	FTEs	Burdened Costs	FTEs	Burdened Costs
BES-funded Operations	101.06	30.31M	145.49	46.30M	182.21	60.81M
Experimental Program	89.01	25.94M	91.27	28.43M	113.40	38.61M
Beamline Development	12.05	4.37M	54.22	17.86M	68.80	22.20M
Other Funded Operations	24.65	8.56M	37.18	12.60M	46.12	14.52M
Experimental Program	20.28	5.96M	22.91	6.52M	27.34	9.62M
Beamline Development	4.37	2.61M	14.27	6.08M	18.78	4.90M

- BES-Funded Experimental Program M&S was 19.1% of total budget for FY2015
- BES-Funded Experimental Program M&S was 18.3% of total budget for FY2016

Staffing Requirements to Support Operations

- Operations requirements are developed through a carefully constructed Work Breakdown Structure (WBS)
- Effort is charged where work is performed so we are able to understand actual costs for each WBS element
- The Experimental Program in Photon Science Division may be separated into 2 distinct categories.
  - Incremental operating effort that **directly scales** with the number of facility-operated beamlines (X-Ray Operations)
  - Operating effort that **doesn't scale** with the number of operating beamlines. This category might weakly scale with the number of users, or might not scale with either number of users or operating beamlines

“Beamline Operations” Budget Components

- BES Beamline Operations
  - **Experimental Program**
    - **Effort that scales with # of beamlines (X-Ray operations)**
    - **Effort that doesn’t scale with # of beamlines**
    - VIPIC
  - Beamline Development
    - Beamlines Developed by NSLS-II (BDN)
    - NSLS-II Partner Beamlines (NPB)
    - Instrument Execution Plan Development (IEPD)
- Other Funded Beamline Operations
  - Experimental Program
    - Strategic Partnership Projects (SPP), SBIR, LSBR
    - LDRD & Program Development
  - Beamline Development
    - Other Funded Work – Partner Beamlines
    - HEX

Experimental Program for FY2016 (BES-Funded)

	FTEs*
Experimental Program total	91.3
X-Ray Operations (scalable)	44.8
Instrumentation Support and R&D	15.0
Facility Controls, Computing and Data	13.4
User Programs	7.6
Engineering, Technical & User Operations Support	7.0
Experimental Management	2.3
Org Burden	1.2

*FTE count based on actual labor charges in FY2016

Actual FY2016 FTE effort per operating beamline

- The 5.54 FTE average in FY2016 for operating ID beamlines is expected to drop to 4.82 FTEs for operating ID beamlines in FY2017.

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

Beamline	Actual FTEs in FY2016
HXN	7.22
SRX	5.25
IXS	5.87
CHX	6.73
CSX-1	4.54
CSX-2	3.67
XPD	5.52
Total	38.8
Average	**5.54**

Effort per BES Beamline in Steady State Ops

Required effort for steady state beamline operations	ID	BM/3PW
	(FTE)	(FTE)
Program Management (.5 FTE for 4-5 beamlines)	0.16	0.16
Admin (1 FTE for 10 beamlines)	0.1	0.1
Beamline Scientists/Professional staff (FTE per beamline)	2.75	2
Beamline Engineering support (1 FTE for 5 beamlines)	0.2	0.2
Beamline Technician Support (1 FTE for 4 beamlines)	0.25	0.25
Mechanical design support (1 FTE for 10 beamlines)	0.1	0.1
Experimental Controls technician (1 FTE for 10 beamlines)	0.1	0.1
Experimental Controls EE (1 FTE for 10 beamlines)	0.1	0.1
Experimental Controls Engineer (1 FTE for 4-5 Beamlines)	0.25	0.2
Software Engineer for DAQ Support (1 FTE for 6-10 beamlines)	0.15	0.1
Comp. Sci for Data Visual & Analysis (1 FTE for 6-10 beamlines)	0.15	0.1
IT prof for Data Storage & Processing (1 FTE for 6-10 beamlines)	0.15	0.1
Mechanical Utilities Engineer (1 FTE for 40 beamlines)	0.025	0.025
Mechanical Utilities Tech (1 FTE for 20 beamlines)	0.05	0.05
Survey Support (1 FTE for 50 beamlines)	0.02	0.02
electrical designer (1 FTE for 25 beamlines)	0.04	0.04
electricians (1 FTE for 30 beamlines)	0.03	0.03
PPS maintenance Engineer (1 FTE for 40 beamlines)	0.026	0.026
PPS maintenance tech (1 FTE for 18 beamlines)	0.054	0.054
Vacuum Engineer (1 FTE for 22 beamlines)	0.046	0.046
Vacuum Tech (1 FTE for 30 beamlines)	0.034	0.034
Total	**4.785**	**3.835**

Benchmarking with APS Experimental Operations

- Visit to APS in December 2015 as requested in 2015 Budget Review to compare WBS and effort levels
- Comparison for actual APS effort in FY2015 vs NSLS-II Steady State plan

Staff not scaled with # BLs	APS	NSLS-II
Management & Admin (Division)	2.04	3
Research Operations Support	3.41	7.75
User Program Support	8.9	6
Nano-positioning	0.99	3.7
Optics	6.1	3.15
Metrology	6.92	3.4
Detectors	8.96	5.1
CAT/Partner support	3.16	5.4
Special Projects	0.93	1
Computing, IT, network infrastructure, data, controls	10.9	12.25
Totals	52.3	50.75

Effort Scaled with # ID BLs	FTEs/BL APS ID	FTEs/BL NSLS-II ID (Steady state)
Program/Group management	0.32	0.26
Dedicated staff at ID beamline	3.58	3
Engineering & Design	0.00	0.3
Computing & Software	0.27	0.45
Controls	0.18	0.45
PSS/BLEPS	0.27	0.08
Maintenance & service	0.11	0.25
Totals	4.73	4.79

Partner User Beamline Support

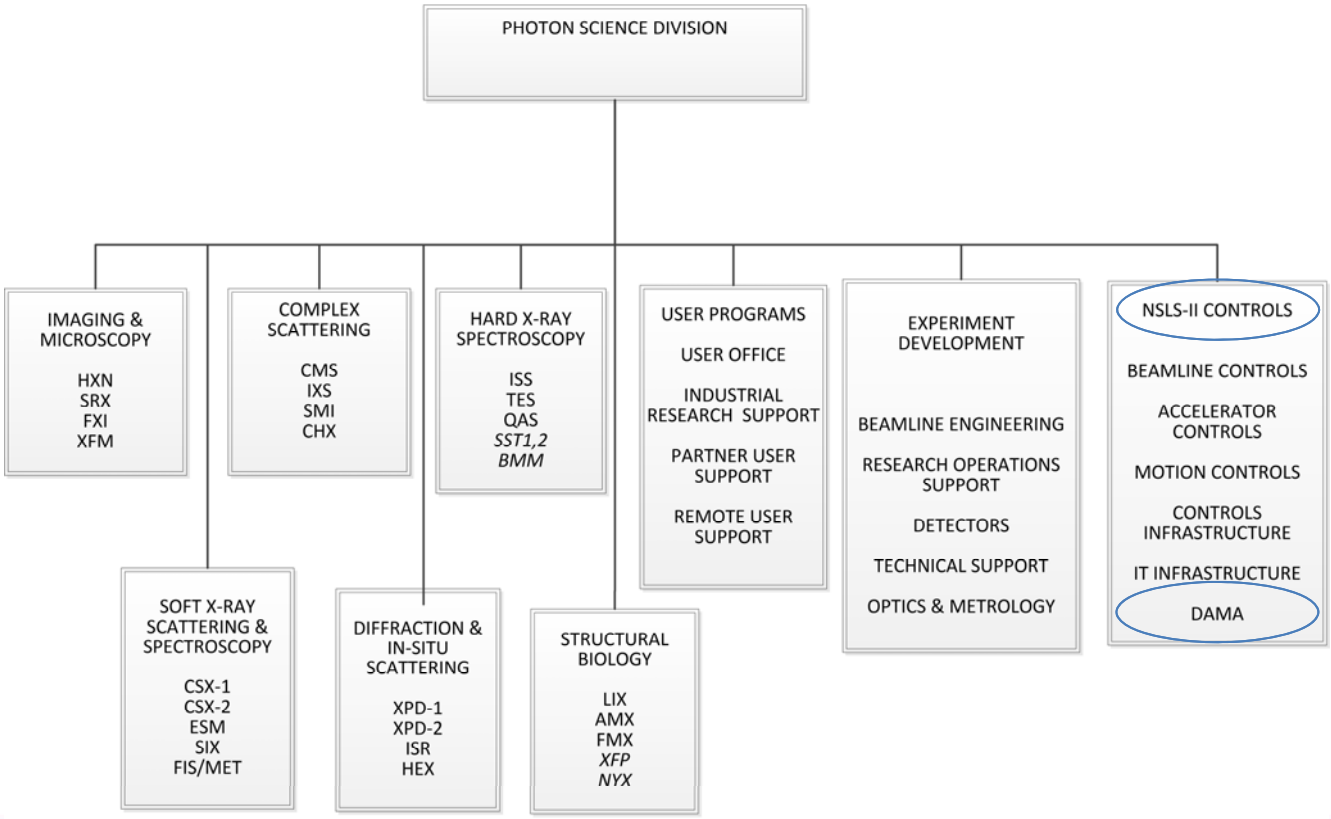
- Support beamline operations on partner-operated beamlines to assure these remain in excellent working condition
- Provide controls effort to encourage standardization using NSLS-II approaches to controls and data handling. (Effort only provided for NSLS-II compliant controls/data approaches).
- This investment in partner-operated beamlines is highly leveraged and positions these beamlines to maximize the number of users and scientific productivity.

Partner-operated support	**ID**
	(FTE)
Experimental Controls, EPS, IT, Network/Data Storage & Processing	0.30
Mechanical Utilities, Survey, Vacuum, PPS support, Electricians, etc…	0.375
Total	**0.675**

EVOLUTION OF ORGANIZATION SINCE 2015

Changes in Photon Science Division Organization

- Controls Program moved to Photon Science Division
- Key staffing recruitments
- Shared science associates across beamline programs



Response to recommendations

- Following the 2014 triennial review, a detailed bottom-up assessment of effort needed to fully exploit NSLS-II project investment and optimally operate beamlines was performed.
- Further revision of x-ray operation effort following BES Operations Review in June 2015.

Reductions relative to 2015 per BL estimate

Steady State ID Beamline Operations	ID Beamline	FTE Delta	% Change
	(2015 estimate)	(Steady state plan)	(Steady state plan)
Beamline Scientist/Professional Staff (FTE per beamline)	3	-0.25	-8%
Beamline Engineering support (1 FTE for 5 beamlines)	0.2	0.02	10%
Beamline Technical Support (1 FTE per 4 beamlines)	0.25		
Mechanical Design Support (1 FTE for 10 beamlines)	0.1		
Experimental Controls Technician (1 FTE for 10 beamlines)	0.1		
Experimental Controls EE (1 FTE for 10 beamlines)	0.1		
Controls Engineer (1 FTE for 3-4 beamlines)	0.3	-0.05	-17%
Controls Engineer for DAQ Support (1 FTE for 3-4 beamlines)	0.2	-0.05	-25%
Comp. Sci. for Data Visual. & Analysis (1 FTE for 3-4 beamlines)	0.3	-0.15	-50%
IT Prof. for Data Storage & Processing (1 FTE for 5-6 beamlines)	0.2	-0.05	-25%
Mech utility maintenance engineer (1 FTE for 20 beamlines)	0.05	-0.025	-50%
Mech utility maintenance tec (1 FTE for 10 beamlines)	0.1	-0.05	-50%
Electrical Designer (1 FTE for 12 beamlines)	0.08	-0.04	-50%
Electrician (1 FTE for 10 beamlines)	0.1	-0.07	-70%
PPS maintenance Engineer/Tech (1 FTE for 12 beamlines)	0.08		
Vacuum Engineer/Tech (1 FTE for 10 beamlines)	0.1	-0.02	-20%
Management & Admin (1 PM/5 beamlines; 1 admin/10 beamlines)	0.3	-0.04	-13%
Total	**5.56**	**-0.775**	**-14%**

Efficiency improvements since FY2015

- Controls program moved to Photon Science Division to better coordinate with operating beamline requirements
- Reduced FTE / beamline from 5.56 to 4.79 in steady state
- Science Associate assignments made at program level for increased efficiency and broader impact across several beamlines
- Cross training technicians initiated to expand individual skill sets
- Scientific staff assist with commissioning across beamlines; talent pool established to aid beamline commissioning
- Student pipeline initiated to address need for controls and software engineers
- Initiated equipment pool for shared instrumentation

FUTURE PLANS

Goals for “Beamline Operations” in FY2018 (1)

NSLS-II source currently holds competitive advantage and aggressive user program ramp-up is needed to fully exploit this advantage for high-impact science

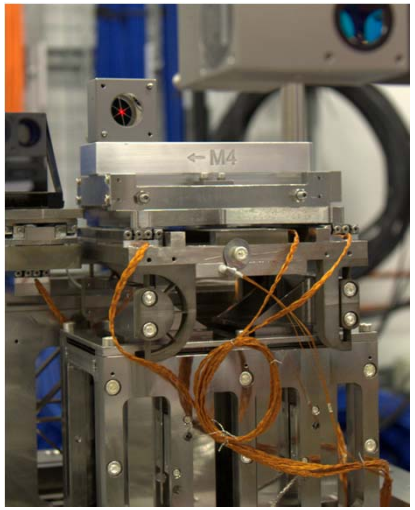
- Maintain safe and productive operations on all beamlines
- Grow Unique User participation and publication output at NSLS-II beamlines
- Complete construction activities on beamlines currently under development
- Continue commissioning for additional capabilities on all 20 BES-operated beamlines
- Continue beamline developments on CDI and HEX; execute R&D toward ARI
- Advance the open-source model for data handling/analysis environment to facilitate user access to data and analysis codes

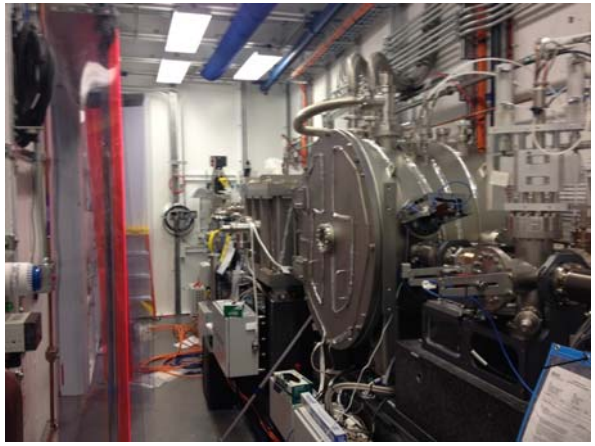
Goals for “Beamline Operations” in FY2018 (2)

- Implement Proposal, Allocation, Safety and Scheduling (PASS) integrated with CFN and other BNL facilities
- Support safe operations of sample preparation and user laboratories for staff and users.
- Maintain detector development program to support NSLS-II beamlines
- Continue development of Multilayer Laue Lens technology for nano-scale focusing applications; implement MLLs with improved spatial resolution
- Deploy nano-positioning advancements to NSLS-II beamlines for sample and optical component positioning requirements
- Extend wavefront simulation framework to include beamline commissioning and virtual beamline experiments.

Adding New Capabilities to Beamlines

- XPD high resolution operation mode
- XPD high pressure – large volume press
- SRX ultra-high spatial resolution operation mode
- CHX multilayer monochromator
- HXN sample temperature environment
- IXS improvements in energy resolution and throughput





SUMMARY

Summary

- Actively managing budget resources to achieve our goals
- Very successful initial ramp-up of beamlines into commissioning and general user operations
- Rapid transition to general user operations with a phased commissioning approach has allowed early scientific results
- R&D investments allow advancement of the R&D program to support and advance NSLS-II beamline performance.
- Improvements have been implemented for more efficient x-ray operations
- The data handling/analysis environment is maturing and has attracted interest at other facilities

“Beamline Operations” Budget and Spending

	FY2015				FY2016				FY2017			
	BES-OPS		Other Funding		BES-OPS		Other Funding		BES-OPS		Other Funding	
Resource	FTEs	Burdened ($K)	FTEs	Burdened ($K)	FTEs	Burdened ($K)	FTEs	Burdened ($K)	FTEs	Burdened ($K)	FTEs	Burdened ($K)
Total	101.1	30,310	24.6	8,563	145.5	46,298	37.2	12,595	182.2	61,167	46.1	14,521
Manager Effort	2.1	746	0.0	0	3.2	1,030	0.0	0	4.4	1,439	0.3	103
Scientist Effort	31.6	9,042	4.5	1,435	41.3	12,136	7.5	2,151	55.7	16,855	9.0	2,993
Engineer Effort	29.4	6,761	8.0	1,665	46.5	10,404	13.6	2,871	63.3	14,066	18.3	3,851
Technical Effort	27.1	4,967	3.7	559	42.2	6,423	11.0	1,586	46.0	7,807	13.9	2,225
Post Doc Effort	2.8	334	7.6	875	3.8	476	5.0	545	3.1	371	4.5	549
Student Effort	-	0	0.3	16	-	0	-	0	0.5	33	-	0
Admin Effort	8.1	1,128	0.5	56	8.6	1,266	0.1	17	9.3	1,439	0.1	17
M&S		6,869		3,799		14,005		5,296		18,218		4,701
Travel		464		158		559		128		940		83