Science and Technology Development at Light Source Facilities Around the World

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Brookhaven National Laboratory

African Light Source Workshop at ESRF, Grenoble, France
November 16-20, 2015

THE AFRICAN LIGHT SOURCE CONFERENCE AND WORKSHOP

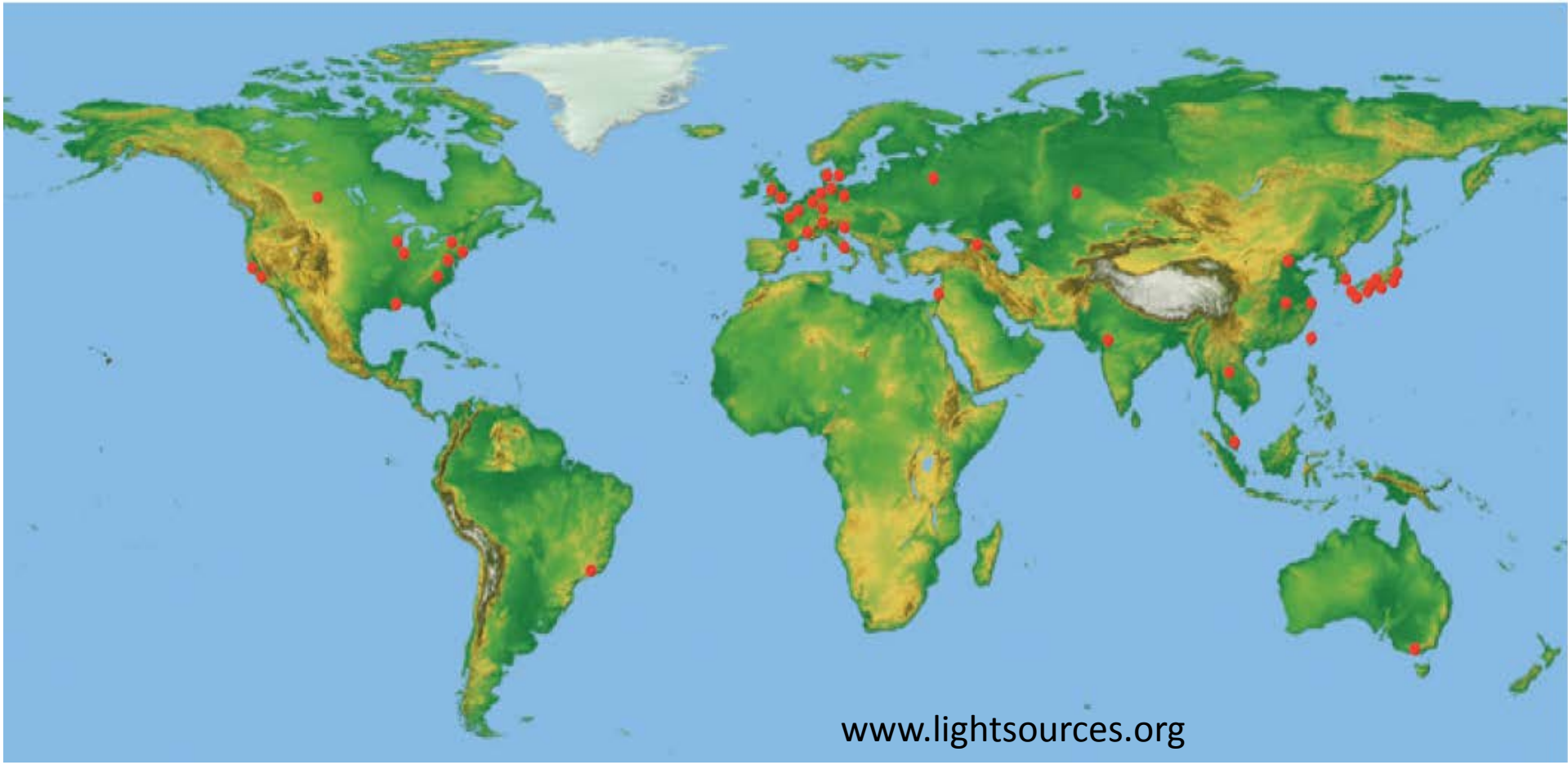
16 - 20 NOVEMBER 2015, ESRF GRENOBLE FRANCE

Outline

- Introduction
- Science & Technology – Perspective from SRI 2015 Conference
- NSLS-II Programs
- Summary Thoughts

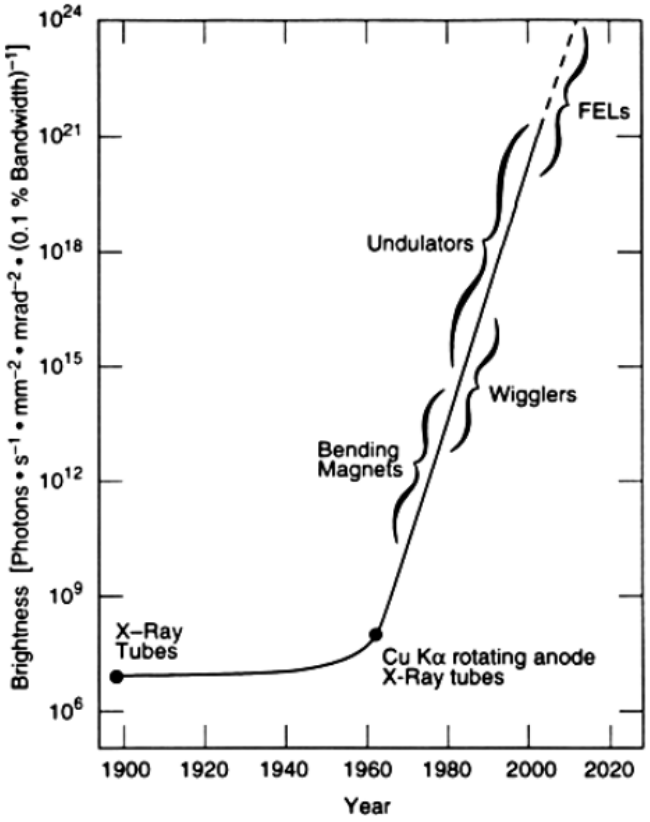
Light Source Facilities Around the World

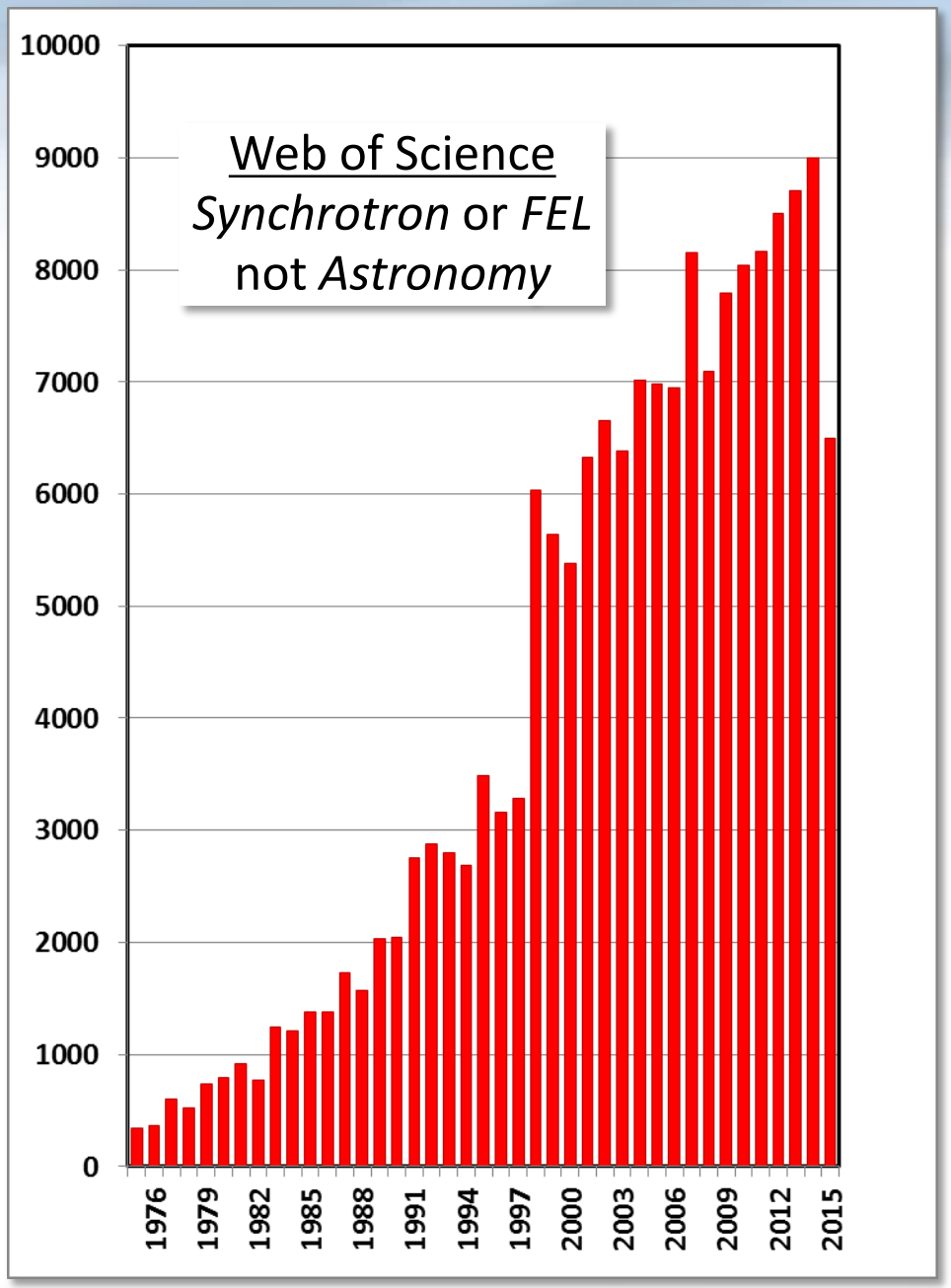
- >47 light source (SR & XFEL) facilities in the world



Growth in Synchrotron Science

- Steady growth in past four decades – big jump in late 1990's fueled by 3rd-SRs





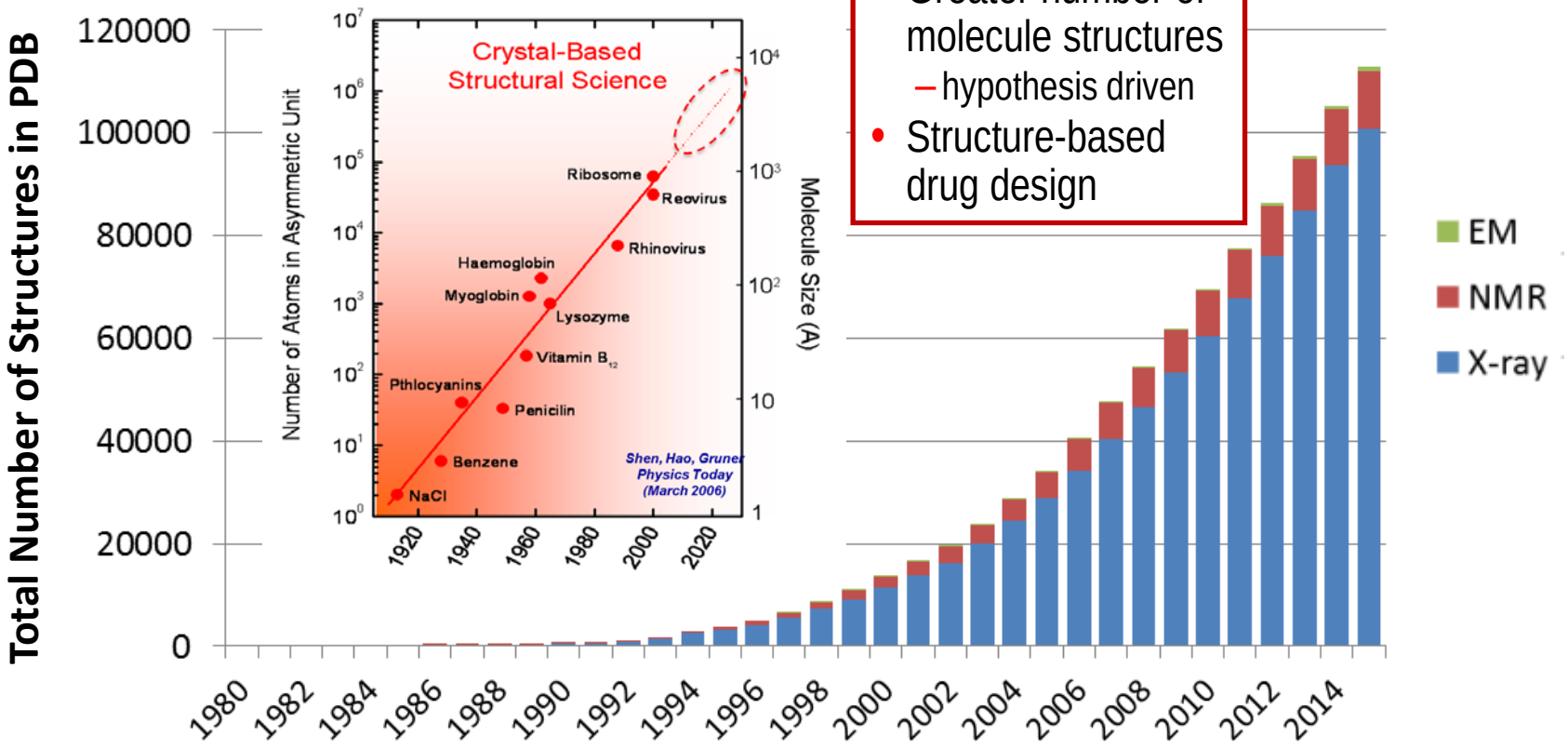
Growth in Synchrotron Based Structural Biology

RCSB PDB PROTEIN DATA BANK — An Information Portal to 113130 Biological Macromolecular Structures

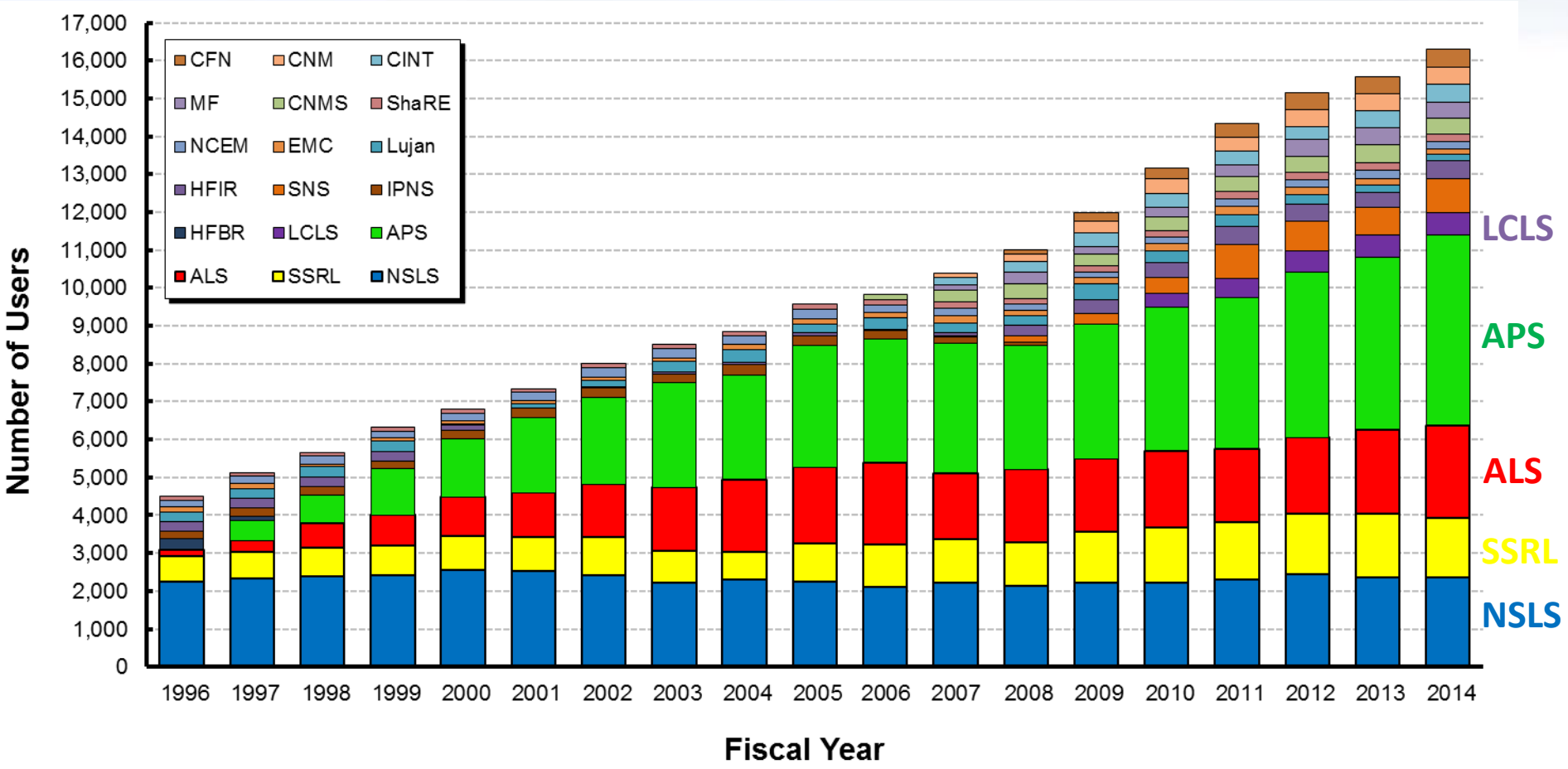
Search by PDB ID, author | Go | Advanced Search | Browse by

PDB-101 | Worldwide PDB | EMDataBank | Nucleic Acid Database | StructuralBiology Knowledgebase

- Larger complexes & membrane proteins
- Greater number of molecule structures
  - hypothesis driven
- Structure-based drug design



US DOE-BES Light Source Facilities Hosted 12,000 Users in FY 2014



More than 300 companies from various sectors of the manufacturing, chemical, and pharmaceutical industries conducted research at BES scientific user facilities. Over 30 companies were Fortune 500 companies.

International Conference SRI
July 6-10, 2015

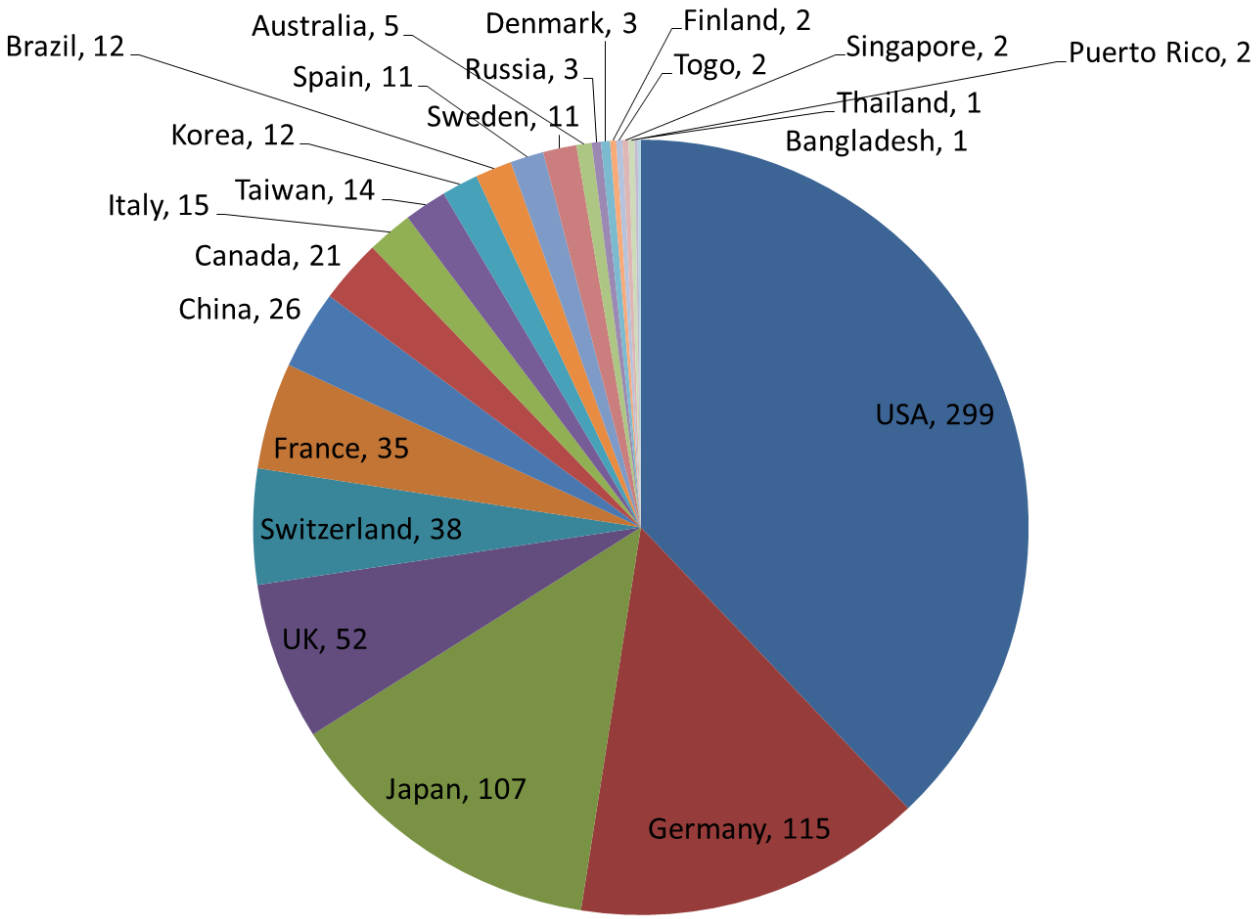
SRI 2015
NEW YORK CITY


Welcome Reception at Broadway Lounge


NSLS-II Tour

U.S. DEPARTMENT OF ENERGY | Office of Science

789 Registered Participants Representing 23 Countries



USA	299
Germany	115
Japan	107
UK	52
Switzerland	38
France	35
China	26
Canada	21
Italy	15
Taiwan	14
Korea	12
Brazil	12
Spain	11
Sweden	11
Australia	5
Russia	3
Denmark	3
Finland	2
Togo	2
Singapore	2
Puerto Rico	2
Thailand	1
Bangladesh	1

Total of 627 Oral & Poster Presentations and 67 Vendor Displays

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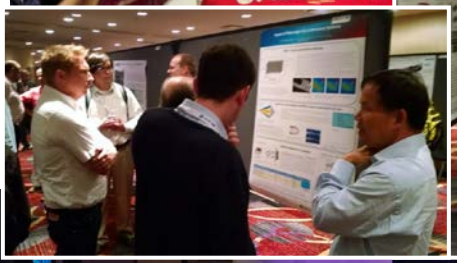
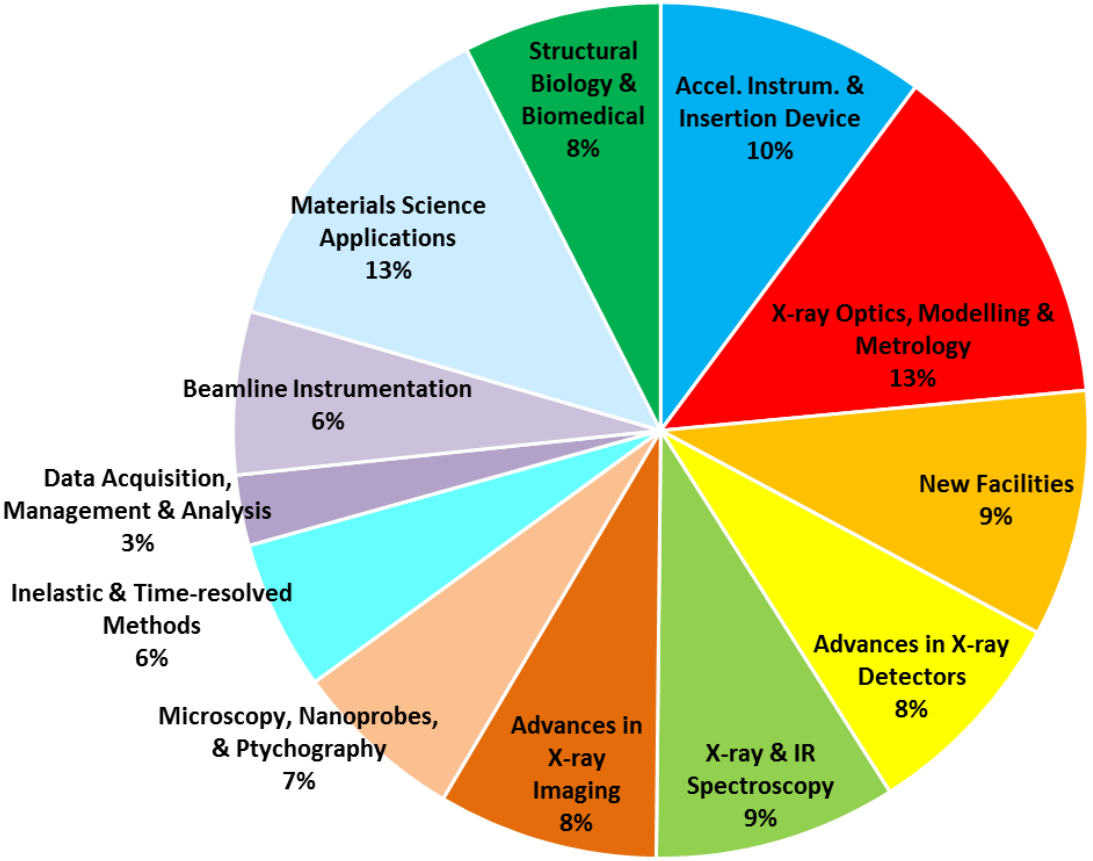


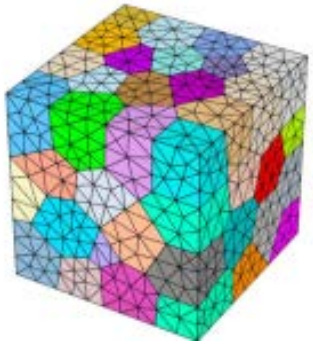
Keynote & Plenary Talks	14
Oral Presentations	175
Poster Presentations	438
Total # of Presentations	627

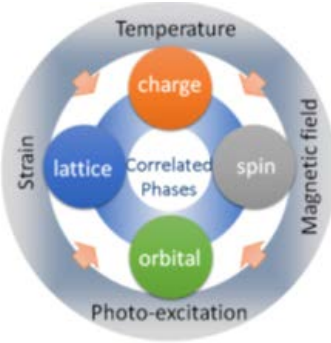


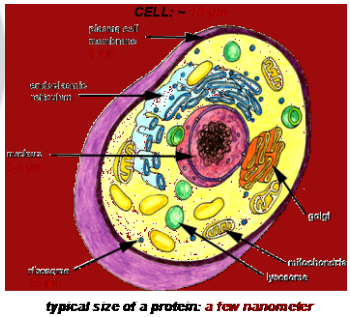
Research Themes in Scientific Applications

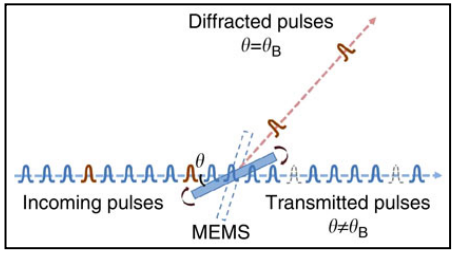
Science Applications:

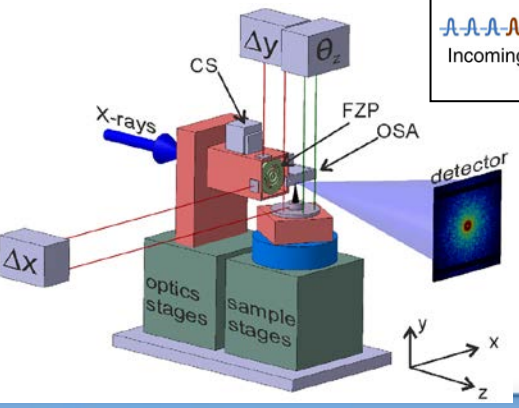
- Functions in real systems
- Complex materials & systems
- Dynamics & kinetics

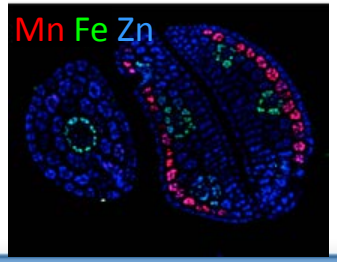












Instrumentation Development:

- In-situ & in-operando methods
- Multi-scale studies & imaging
- Inelastic & time-resolved methods

Keynote & Plenary Presentations

– *along science or instrumentation themes*

<u>Tuesday</u>: In-situ/operando Materials Science & Industrial Applications

- Matthew Miller (Cornell University): Understanding the Crystal Scale Performance of Structural Materials
- Ho-kwang Mao (HP-STAR): Materials Discovery at High Pressures in Earth and Energy Sciences
- Masaki Takata (Tohoku University): Industry Research Program at SPring-8

<u>Wednesday</u>: Biological Applications, X-ray Imaging & Microscopy

- Henry Chapman (DESY): Serial Crystallography at Free-Electron Laser and Synchrotron Light Sources
- Eva Pereiro (ALBA): Cryo Soft X-ray Tomography for Elucidating Pathogen-Cellular Interactions
- Yong Chu (NSLS-II): The New Nanoprobe for Hard X-rays

Industrial Research at SPring-8

Masaki Takata (Tohoku University)

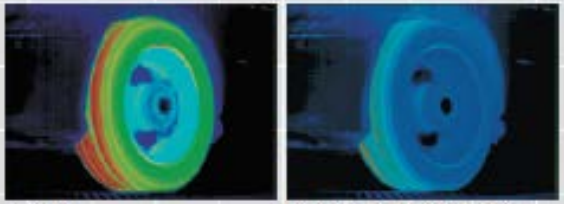
Achievements

- Development of a **time resolved two-dimensional ultra-small-angle X-ray scattering technique (2D-USAXS)** that can measure the three-dimensional structural information of silica nanoparticles in the rubber of tires
- By combining 2D-USAXS with **time resolved two-dimensional small angle X-ray scattering (2D-SAXS)***, development of a new material using molecular design based on the results of the two analyses
- Commercialization of high performance tires, with **rolling resistance**** reduced by 39% and fuel-efficiency improved by about 6% compared with their predecessors

Research and development institution : Sumitomo Rubber Industries, Ltd.

Thermographic capture comparing the temperatures of the tire surfaces when driving

Much of the former tire is orange and yellow, indicating high temperatures. The low temperature of the new product reflects its excellent mileage performance.



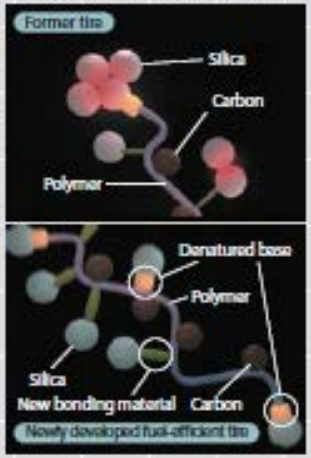
Former tire | Newly developed fuel-efficient tire

Time resolved two-dimensional ultra-small-angle X-ray scattering (2D-USAXS)

A method for measuring the size and shape of structures in the submicrometer range (10^{-7}m) within substances. By making the 160 m long vacuum path of the BL20XU the camera length, it was possible to observe X-rays scattered at an extremely low angle of less than 1/100,000 to analyze the structures in this range. As a result, we could identify the network structure formed by the silica particles in the rubber.

Comparison of the molecular bonds in rubber

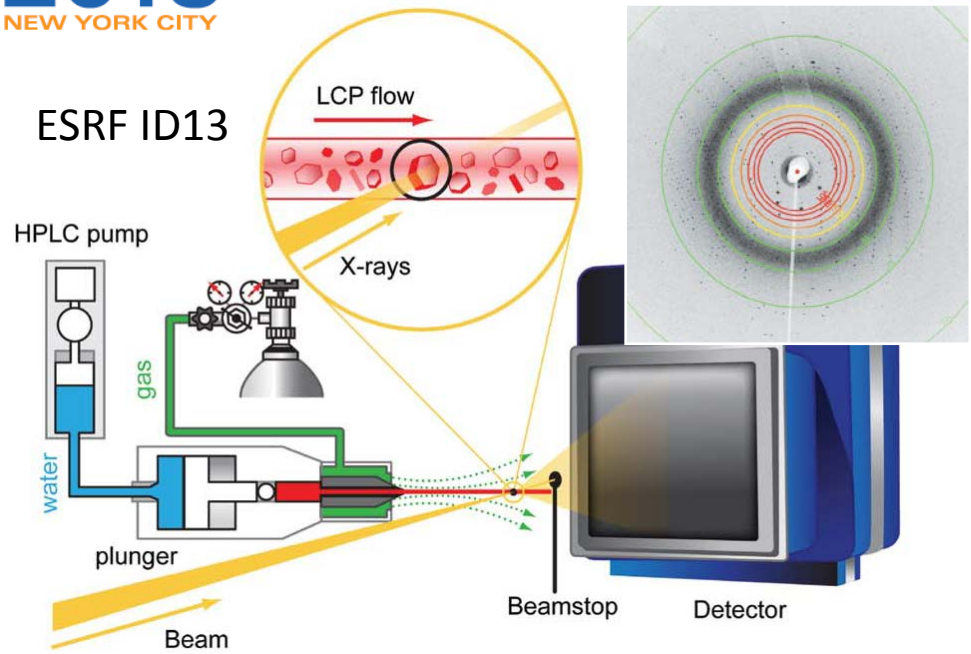
The rubber of tires is composed of synthetic rubber, natural rubber and a stiffener. In the former tires (top), there are few links, which is a factor in heat generation. In addition, the silica coheres to form a network structure. In the new product (bottom), a "both-ends-modified polymer" is used as the synthetic rubber. The denatured bases at the ends of the polymer and the new bonding material work to improve the bonding power of the silica and polymer, and to increase the dispersibility of the silica.

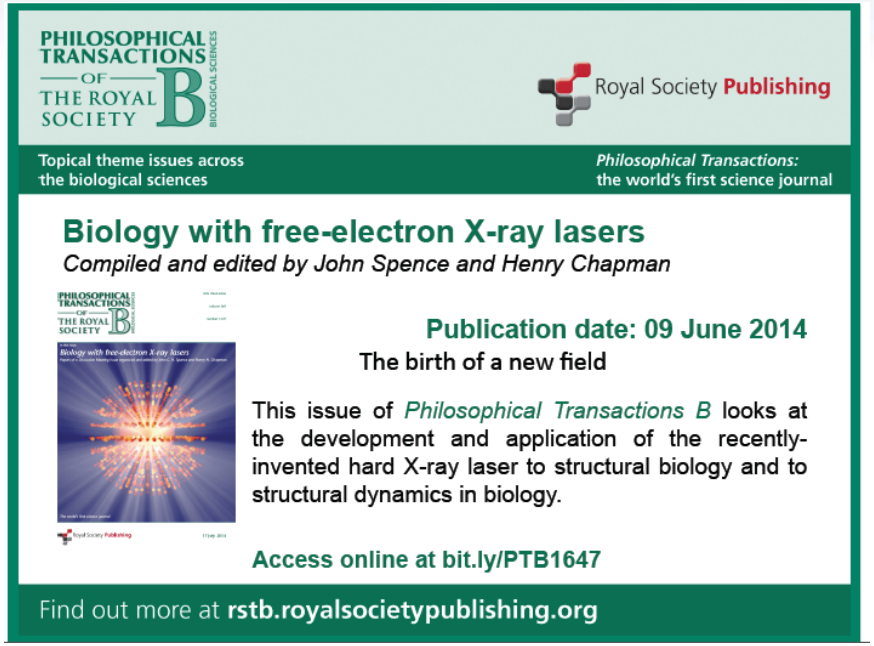


Serial Crystallography at XFEL and SRs

Henry Chapman (DESY)

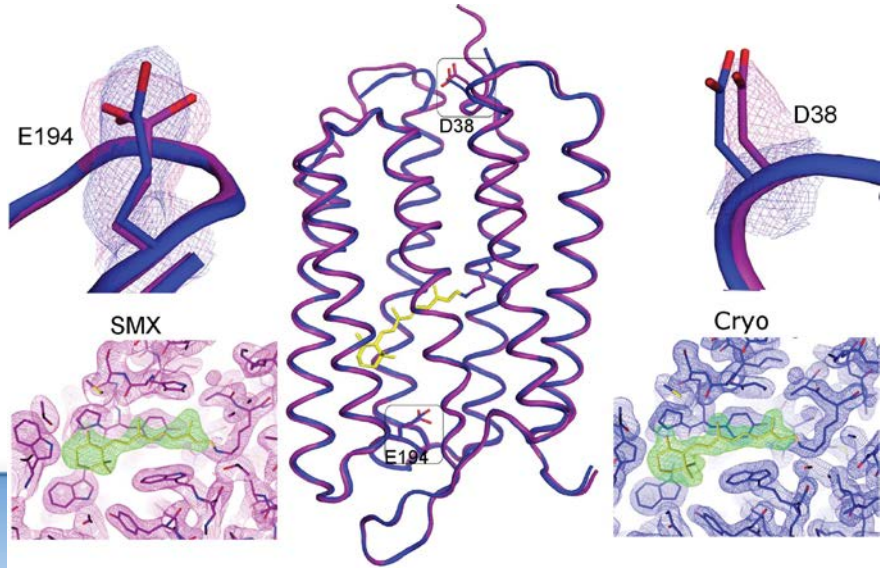
ESRF ID13





- Lipidic Cubic Phase (LCP) based microjet to deliver tiny protein crystals through the X-ray beam; Data collected at RT
- Bacteriorhodopsin (bR) used to compare RT data (purple) with cryo data (blue) from SLS
- Other RT crystal delivery methods possible


[Kisselman, 2011]



Keynote & Plenary Presentations

– *along science or instrumentation themes*

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<u>Thursday</u>: New Facilities, Ultrafast, and Coherent Applications

- Shunsuke Nozawa (KEK): Direct Observation of Bond Formation by Femtosecond X-ray Solution Scattering
- Daniel Ratner (SLAC): Seeded Free-Electron Lasers and Applications
- Ana Diaz (PSI): Development of Ptychographic Tomography for Scientific Applications
- Mikael Eriksson (MAX IV): The Multi-Bend Achromat Storage Rings

<u>Friday</u>: Time-Resolved & Inelastic Applications, and 'Big Data'

- Gopal Shenoy (APS): Measuring the Pathways to Complex Matter Far-From-Equilibrium: Development of Synchrotron X-ray Spatiotemporal Tools
- Nick Brookes (ESRF): Synchrotron Research using Soft X-ray Resonant Inelastic Scattering
- Alexander Föhlisch (HZB): Implications of Adding Dimension of Time & Stimulated Processes to Science with X-rays
- Dilworth Parkinson (ALS): Real-time Data-Intensive Computing

Multi-Bend Achromat (MBA) Storage Rings

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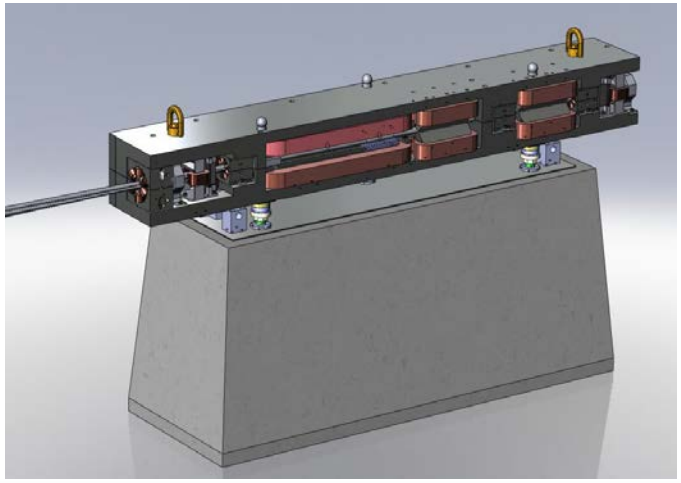
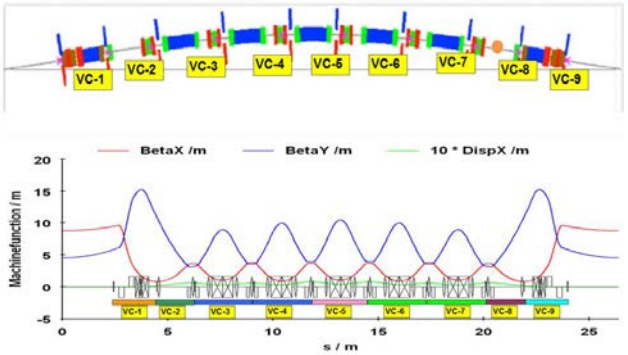
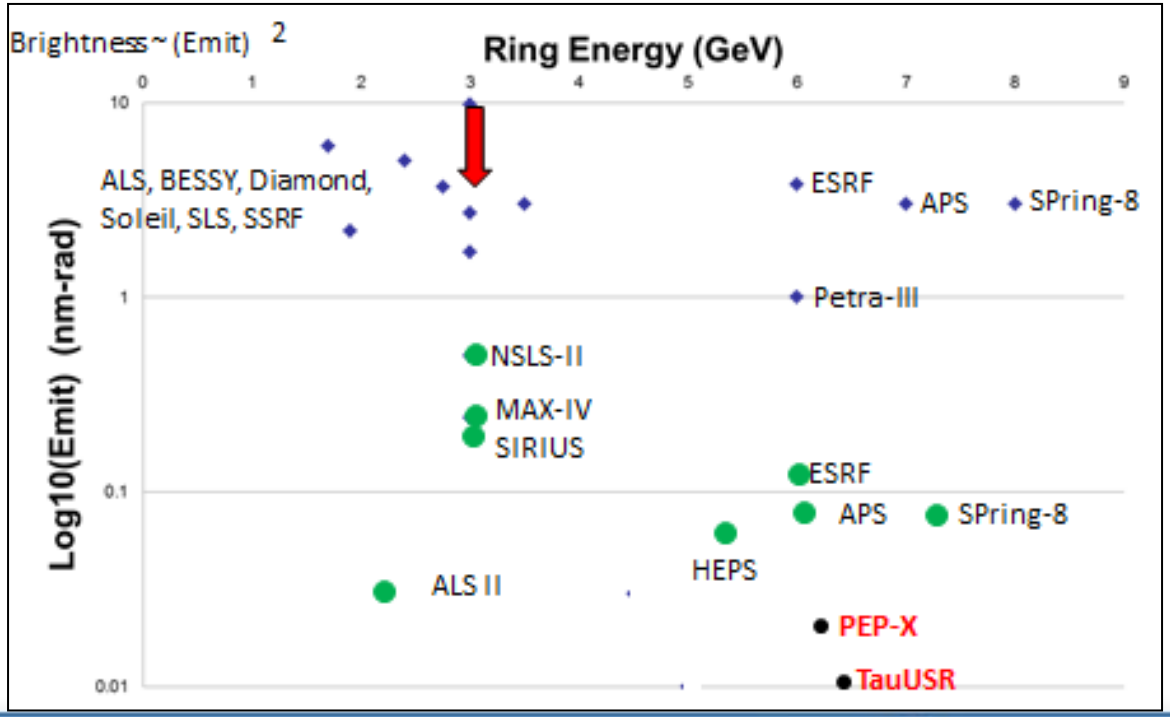
Mikael Eriksson (MAX-IV)







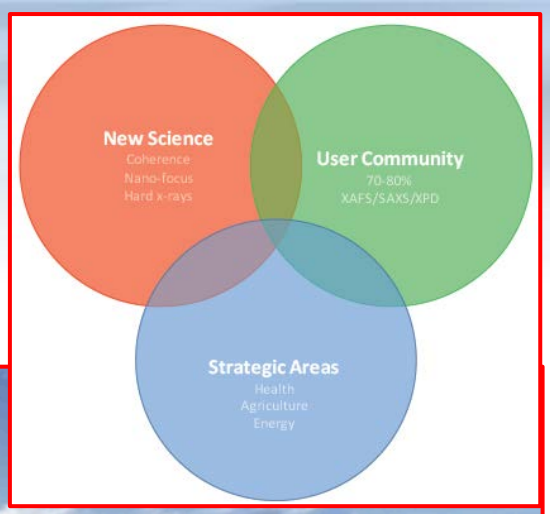
Special Session – New Facilities

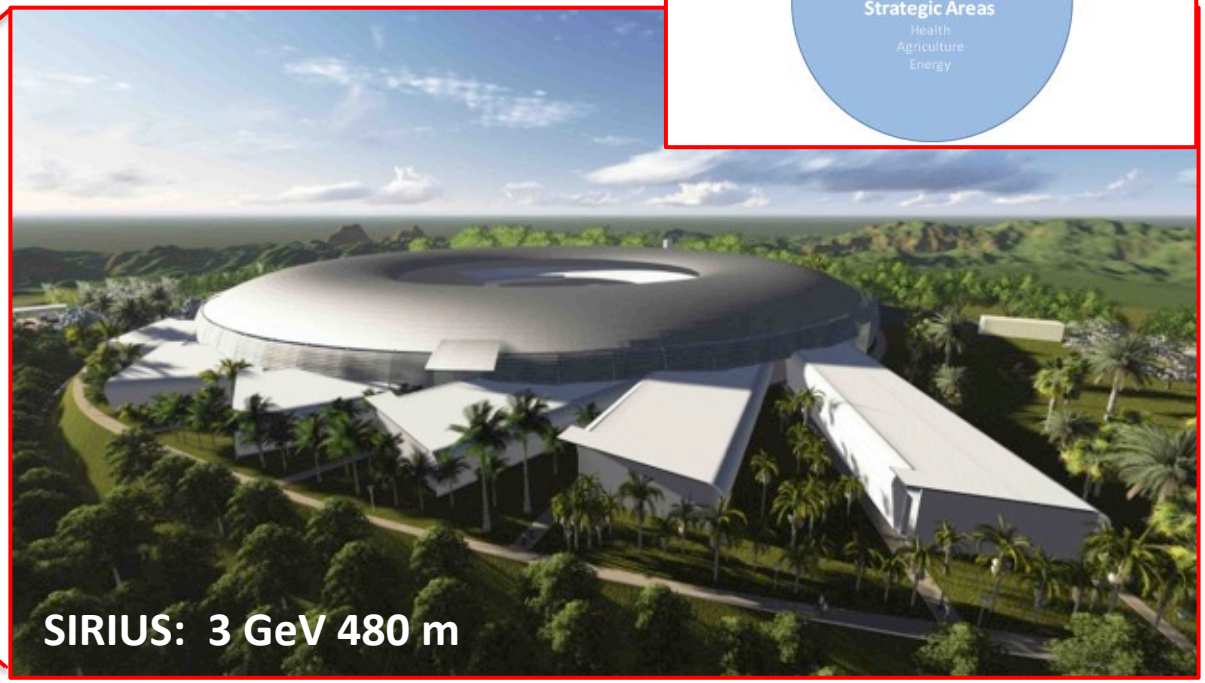
– *New or substantially upgraded facilities*

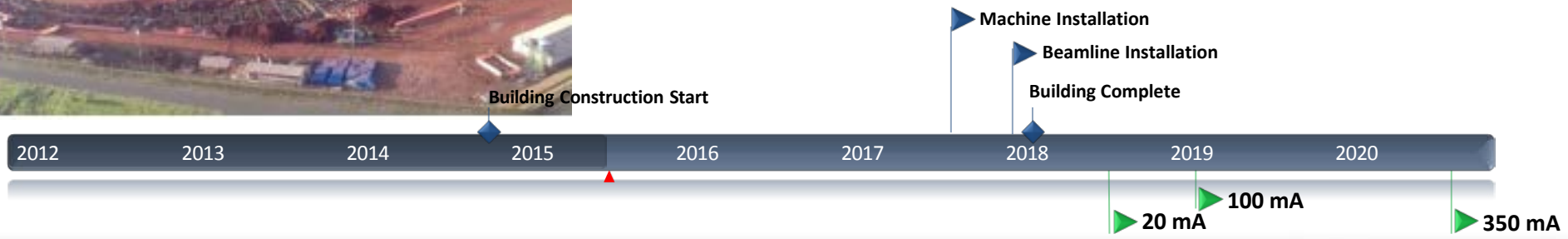
- C. Callegari (FERMI): The FERMI Seeded-FEL Facility – Status and Perspectives
- G. Wang (NSLS-II): Results of the NSLS-II Commissioning
- K. Scheidt (ESRF): Status of the ESRF's new Low-Emittance Storage Ring
- J. Brock (CHESS): New Capabilities at Cornell High Energy Synchrotron Source
- O. Seeck (PETRA-III): PETRA III: Experiments at a low emittance 6 GeV synchrotron radiation source
- S. Gwo (NSRRC): Taiwan Photon Source: Current Status and Future Perspectives
- T. Tschentscher (XFEL): Status of Euro-XFEL
- F. Loehl (PSI): Status of SwissFEL, the X-ray free-electron laser at PSI
- C-J. Yu (PAL): Current status of PLS-II beamlines
- E. Ploenjes (DESY): FLASH2: Operation, Beamlines, and Phonton Diagnostics
- H. Westfahl (SIRIUS): Sirius: the new Brazilian Synchrotron Light Source

SIRIUS – New Brazilian Synchrotron Facility

H. Westfahl (CNPEM)



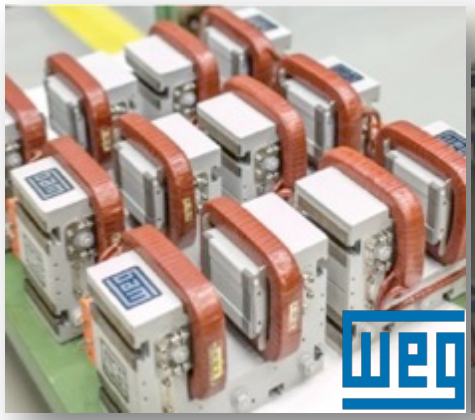


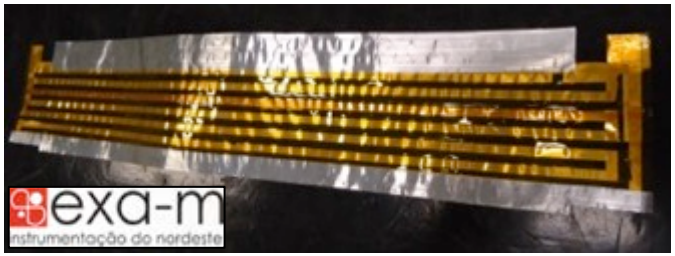


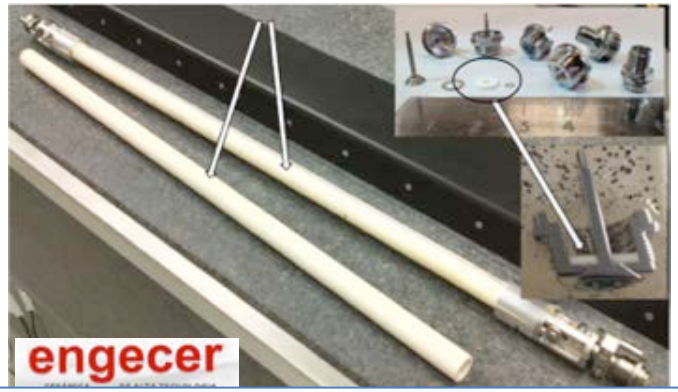
Opportunities to Enhance Capabilities of Brazilian Industries

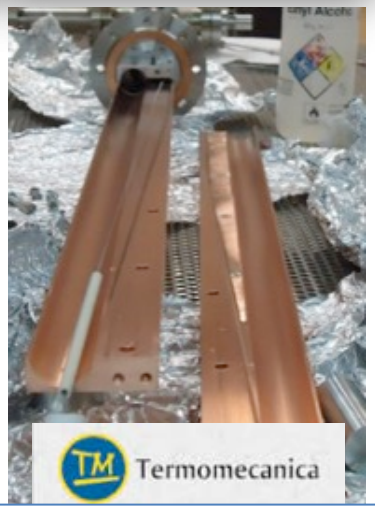
- Continuous interaction with many Brazilian companies in order to find developers as well as suppliers for production

- WEG – magnets (Jaraguá do Sul, SC);
- EXA-M – vacuum baking tapes (Salvador, BA);
- Termomecânica – Cu/Ag alloy for vacuum (São Bernardo do Campo, SP) ;
- Engecer – special ceramics chambers (São Carlos, SP)
- FCA Brasil – vacuum chambers (Campinas, SP)









physicstoday September 2014

"This is the first time in Brazil that we have a major facility project associated with an active effort that will offer R&D funds in a structured manner for small companies to perform research and to develop parts and processes," says Carlos Henrique de Brito Cruz, scientific director of FAPESP

National Synchrotron Light Source II

NSLS-II: newest SR into operations

Storage ring: 792 m, 3 GeV, 500 mA

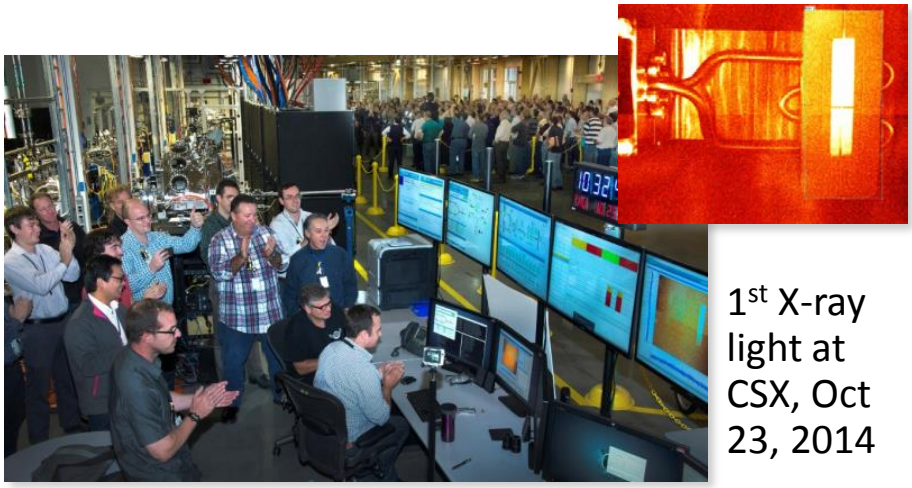
Small e-beam source:

σ_y = 2.6 μm, σ_x = 28 μm,
σ'_y = 3.2 μrad, σ'_x = 19 μrad

Photon energy: from IR to hard X-rays

Capacity: >60 simultaneous experiments

Visiting users: > 4000 per year



1st X-ray light at CSX, Oct 23, 2014

NSLS-II Strategic Planning

- NSLS-II strategic planning process over the past decade identified NSLS-II strengths:
  - World-leading features in low-emittance, high brightness, broad spectrum range, large capacity for medium GeV rings, long beamlines, and stability
  - Advanced beamlines with cutting-edge optics, detectors, and instrumentation, along with excellent expert staff with experience at NSLS and at other facilities worldwide
  - Ideally located in vibrant Northeast US where a strong and experienced community already exist, both in academia & in industry:
    - highly engaged and productive for past 32 years at NSLS
    - strong interests in developing new science programs and partnerships at NSLS-II
    - world-renowned universities and industries – including 7 universities in the US top-ten, and Fortune 500 companies including Pfizer, Merck, Bristol-Myers, Honeywell, Corning, DuPont, GE, IBM, Exxon-Mobile
    - strong and engaged BNL and regional community in science departments and CFN with interests in leveraging NSLS-II in their research programs

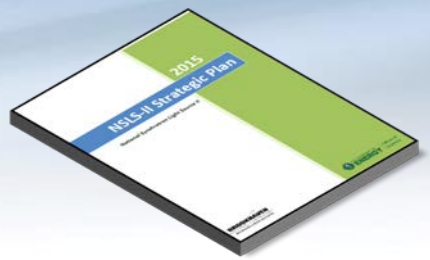
FY13 EFRC Location Map

NSLS-II Vision

- NSLS-II vision is to be an internationally renowned synchrotron facility with world leading capabilities enabling a broad range of high-impact and discovery-class science and technology programs

- High impact:
  - Enable discoveries in science and technology
  - Support research pipeline from discovery to development & deployment

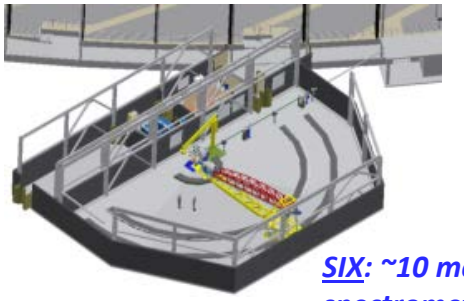
Crosscut Science Themes and NSLS-II Strategic Directions



– 2015 NSLS-II Strategic Plan

- Complexity and Dynamics:

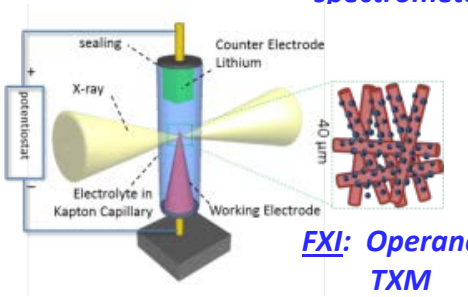
  Strategic Direction 1: Develop world-leading capabilities in high-spatial-resolution nanoprobe and imaging, high-coherent-flux coherent scattering, and high-resolution inelastic scattering



***SIX*: ~10 meV spectrometer**

- In-situ and In-operando Research:

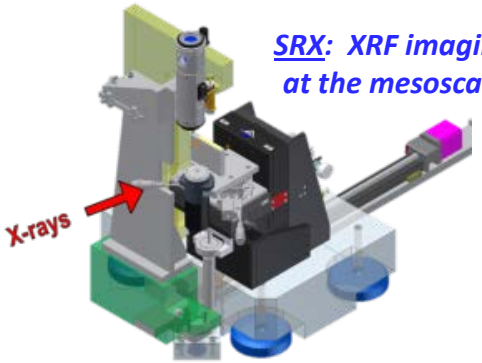
  Strategic Direction 2: Leverage strengths and expertise in the existing scientific and industrial community to develop world-class in-situ and in-operando capabilities



***FXI*: Operando TXM**

- Mesoscale & Multiscale Science:

  Strategic Direction 3: Develop a set of most-advanced, correlative, multi-scale structural and chemical imaging capabilities as well as theoretical and modelling tools in mesoscale and multiscale sciences

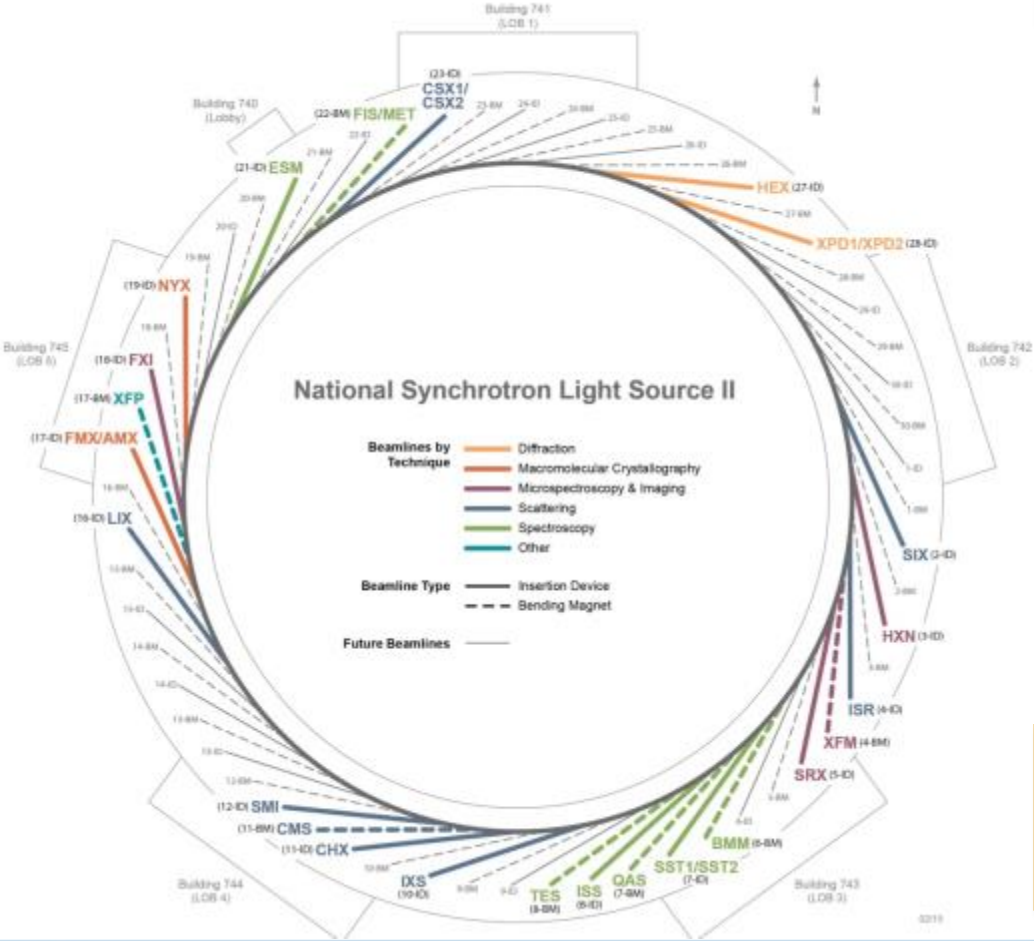


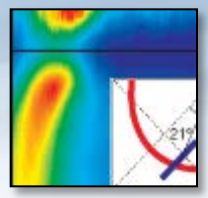
***SRX*: XRF imaging at the mesoscale**

NSLS-II
Current Suite of Beamlines

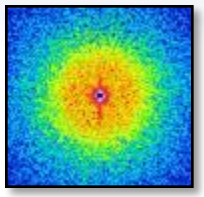
- 7 Operating
- 21 Under Development

http://www.bnl.gov/ps/nsls2/beamlines/map.php

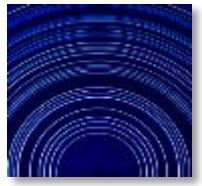




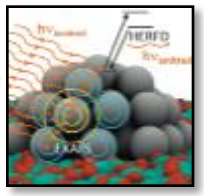
Soft X-Ray Scattering & Spectroscopy
23-ID-1: Coherent Soft X-ray Scattering (2015)
23-ID-2: Soft X-ray Spectr & Polarization (2015)
21-ID: Photoemission-Microscopy Facility (2017)
2-ID: Soft Inelastic X-ray Scattering (2017)
22-BM: Magneto, Ellips, High-P Infrared (2018)



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 (2020)

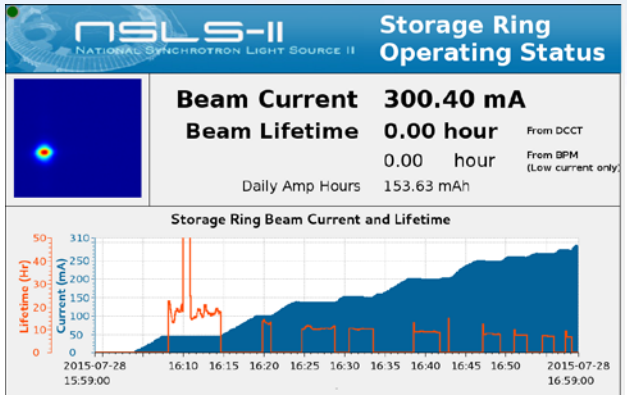


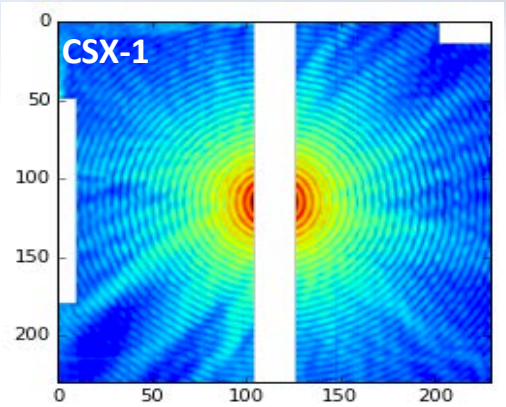
Hard X-Ray Spectroscopy
8-ID: Inner Shell Spectroscopy (2017)
7-BM: Quick X-ray Absorption and Scat (2016)
8-BM: Tender X-ray Absorption Spectr (2017)
7-ID-1: Spectroscopy Soft and Tender (2017)
7-ID-2: Spectroscopy Soft and Tender (2017)
6-BM: Beamline for Mater. Measurement (2017)

Imaging & Microscopy
3-ID: Hard X-ray Nanoprobe (2015)
5-ID: Sub-micron Resolution X-ray Spectr (2015)
4-BM: X-ray Fluorescence Microscopy (2017)
18-ID: Full-Field X-ray Imaging (2018)

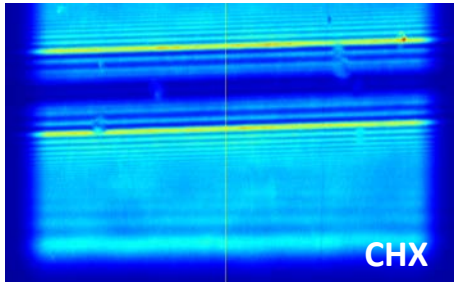
Structural Biology
17-ID-1: Frontier Macromolec Cryst (2016)
17-ID-2: Flexible Access MacromolCryst (2016)
16-ID: X-ray Scattering for Biology (2016)
17-BM: X-ray Footprinting (2016)
19-ID: Microdiffraction Beamline (2017)

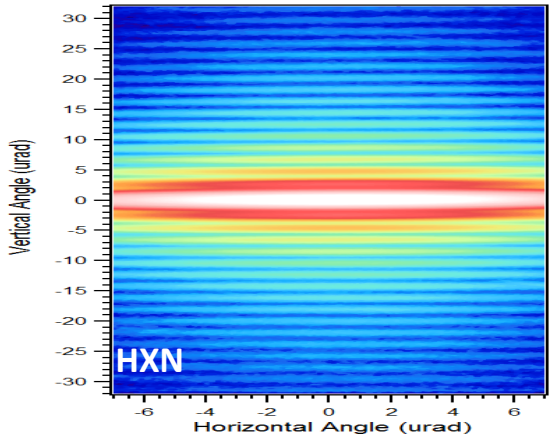
NSLS-II Commissioning & First Users





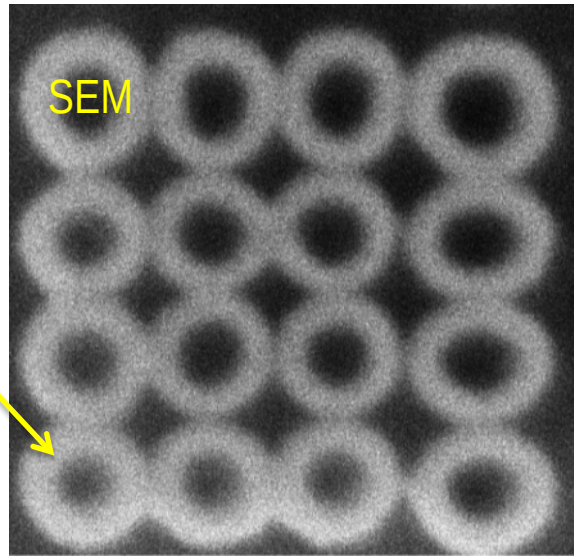
- NSLS-II Project CD-4 approval, March 19, 2015
- First general user – Sunil Sinha (UCSD), July 24, 2015
- All project beamlines routinely operating at 150 mA with top-off; 200 mA expected soon
- All project beamlines conducting user-assisted science commissioning or general user (GU) operations
- Six of the seven project beamlines entering into GU operations in 2015; First publication, Feb. 2015
- Structural biology beamlines starting technical commissioning in 2016; NEXT beamlines to follow





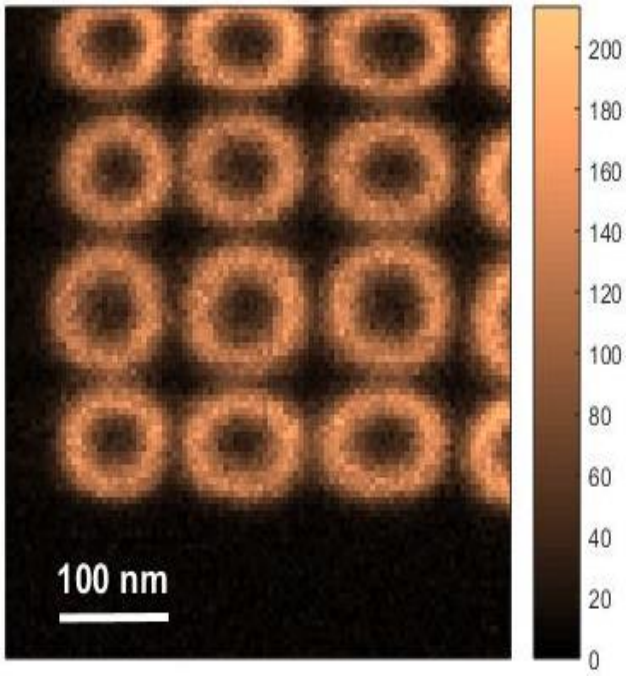
HXN: Fly-scan Nano-Imaging at 15 nm Resolution

Pt test pattern (200 nm thick)
(made by M. Liu, CFN)



20 nm wide

HXN: 12 keV @ 50 mA current

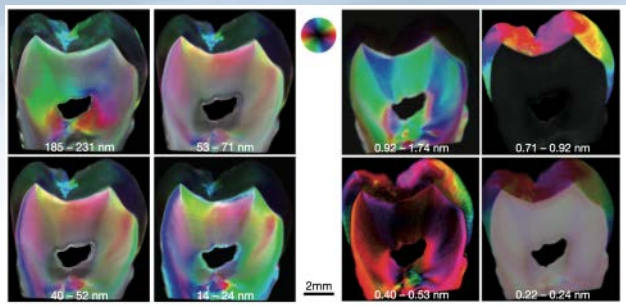


Pt XRF fly-scan: 5nm/pixel

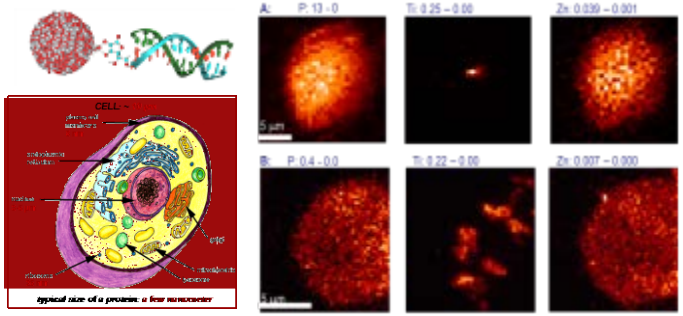
Dwell time: 0.5s/pixel

Resolution: ~15 x 15 nm (FWHM),
~11 x 13 nm (PDS, based on cutoff frequency)

Integrated Tools for Multi-scale Bioscience

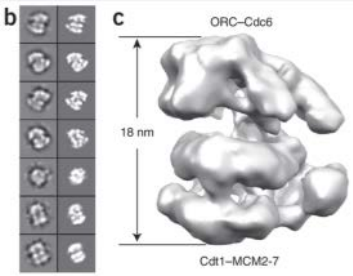


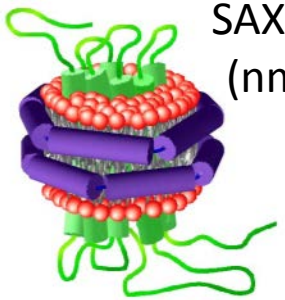
X-ray Imaging (<µm scale)



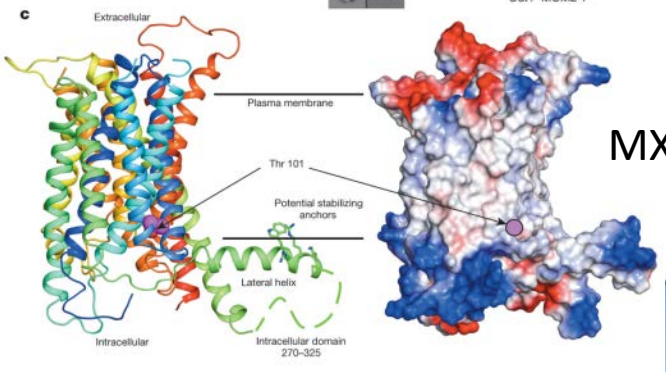
X-ray Microscopy (10-100nm scale)

Cryo-EM (nm scale)





SAXS/WAXS (nm scale)

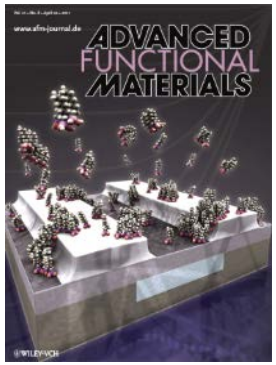


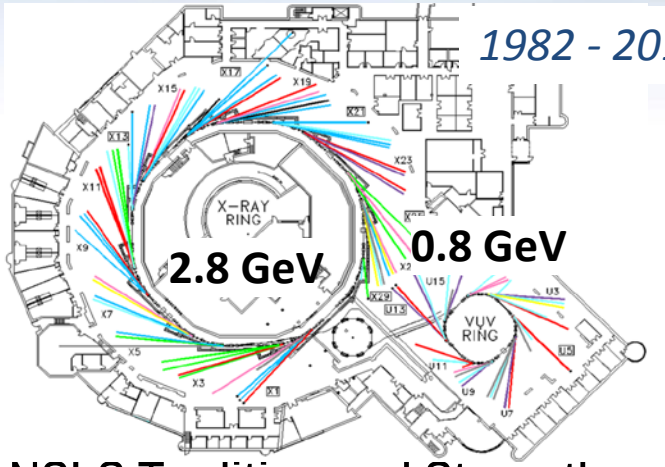
MX (atomic scale)

<u>Multiscale Biosciences at NSLS-II</u>:

- Develop & provide integrated X-ray and complementary tools across multiple length scales along with tools for data handling and integration

NSLS – Three Decades of Science & Impact



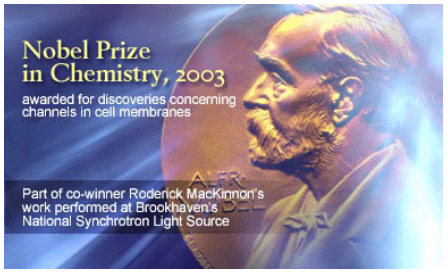


1982 - 2014

- NSLS Tradition and Strengths:
  - Broad range of science programs
  - Diverse capabilities in broad spectral range
  - Highly engaged and productive user community
- Highly Productive & High Impact

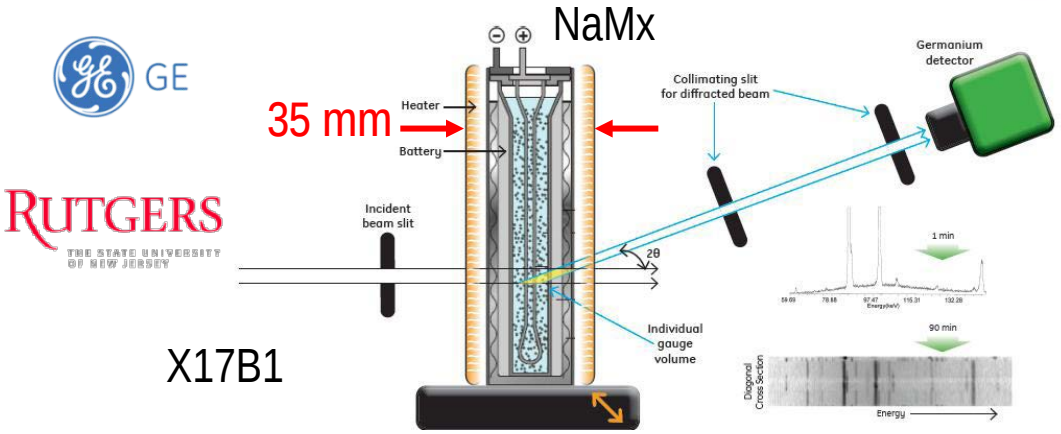
	FY13	Since 1982
• Users	2,367	~ 57,000
• Publications	881	17,182
• Protein Databank Deposits	~ 600	7,122
• 2 Nobel Prizes (2003, 2009)		

- Crucial Resource
  - Universities: SBU, Columbia, MIT, Yale, Rutgers, ...
  - Industry: IBM, ExxonMobil, GE, Pharmaceuticals, ...
  - BNL: CFN, CMP, Catalysis, Biology, Environ Sci, ...



Enabling Innovation through Academia-Industry-Government Collaboration

J Rijssenbeek, Y Gao, Z Zhong, M Croft, N Jisrawi, A Ignatov, T Tsakalakos, *J. Power Sources*, 196, 2332–2339 (2010).



Impact

- Full-size commercial cells probed during cycling
- Unprecedented insight:
  - Chemical distribution
  - Reaction products
  - Conversion rates
  - Degradation pathways
- Fundamentals to guide new product development leadership
- Unique capability: applicable to all battery chemistries

"Our collaborations with the National Synchrotron Light Source have helped to improve our fundamental knowledge and in turn have allowed us to realize significant gains in battery performance. These advancements are foundational to our new business and our ability to bring leadership technology to market."

Glen Merfeld, Energy Storage Leader, GE Global Research

GE DURATHON MANUFACTURING
Schenectady, NY

NSLS: Far-Reaching Science and Impact Can Be Summarized in Several Areas – beyond numbers

- People: NSLS role in development of today's leaders and training of today's scientists
- Science: Experiments pioneered for the 1st time at NSLS that laid foundation for advances today
- Technology: Synchrotron technologies developed at NSLS that are widely used today
- Partnership with Industry: Strong involvement by industry R&D early set the stage for more & continued involvement
- Community: NSLS role in development of today's light source communities

Summary

- Synchrotron light source science and technology is fast evolving research and development field worldwide
- Strong, increasing development trends in complex, real systems at conditions and environment of practical and industrial relevance
- NSLS-II commissioning progressing well and starting user operations now; ramping up to 28 beamline operations by 2019
- Impact of synchrotron well beyond science publications, especially in bringing communities together, in training of students & young scientists, and in industry R&D and economic impact
- AfLS would be a fantastic venue to bring African communities together to realize all these benefits

Thank you for your attention!