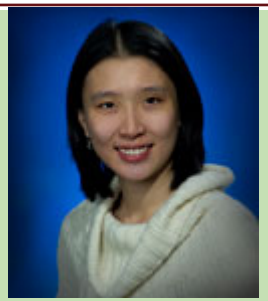
Workshop 1:
Multi-dimensional and Multi-modal X-ray Imaging & Analysis

Organizer(s):



Karen Chen-Wiegart
Stony Brook U.
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Lisa Miller
NSLS-II, BNL

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NSLS-II, BNL

Juergen Thieme
NSLS-II, BNL

Thomas Caswell
NSLS-II, BNL

Stuart Campbell
NSLS-II, BNL

X-ray Imaging & Microscopy Program

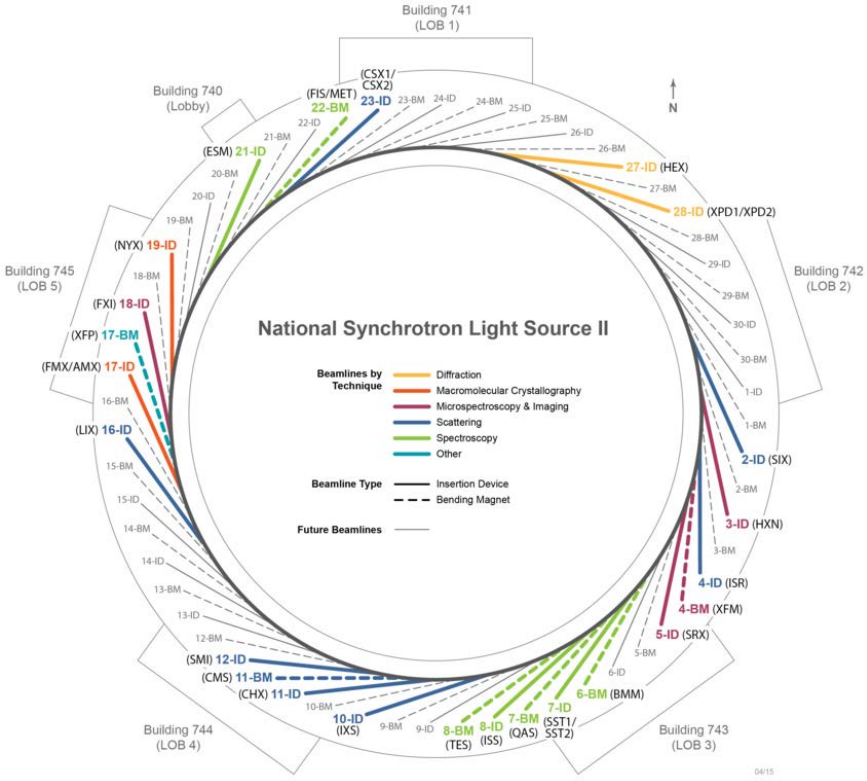
Data Acquisition, Management & Analysis Group

Multi-modal Task Force

Community – Facilities, Users, & Developers!

Motivation - status

NSLS – II Beamlines



Hard X-Ray Spectroscopy

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

Imaging & Microscopy

3-ID (HXN): Hard X-ray Nanoprobe (operating)
5-ID (SRX): Sub-micron Resolution X-ray Spectr (operating)
4-BM (XFM): X-ray Fluorescence Microscopy (2017)
18-ID (FXI): Full-Field X-ray Imaging (2018)

Structural Biology

17-ID-1 (FMX): Frontier Macromolec Cryst (2016)
17-ID-2 (AMX): Flexible Access Macromolec Cryst (2016)
16-ID (LIX): X-ray Scattering for Biology (2016)
17-BM (XFP): X-ray Footprinting for Bio Macromolecules (2016)
19-ID (NYX): Microdiffraction Beamline (2017)

Soft X-Ray Scattering & Spectroscopy

23-ID-1 (CSX-1): Coherent Soft X-ray Scattering (operating)
23-ID-2 (CSX-2): Soft X-ray Spectr & Polarization (operating)
21-ID (ESM): Photoemission-Microscopy Facility (2017)
2-ID (SIX): Soft Inelastic X-ray Scattering (2017)
22-BM (FIS/MET): Magneto, Ellips, High-P Infrared (2018)

Complex Scattering

10-ID (IXS): Inelastic X-ray Scattering (operating)
11-ID (CHX): Coherent Hard X-ray Scattering (operating)
11-BM (CMS): Complex Materials Scattering (2016)
12-ID (SMI): Soft Matter Interfaces (2017)

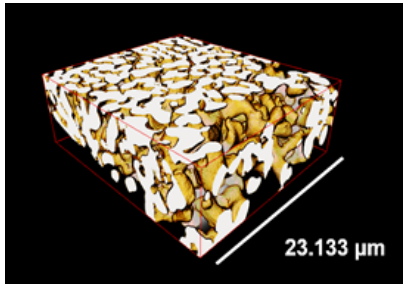
Diffraction & In Situ Scattering

28-ID-1 (XPD-1): X-ray Powder Diffraction (operating)
28-ID-2 (XPD-2): X-ray Atomic Pair Distribution Function (2017)
4-ID (ISR): In-Situ & Resonant X-Ray Studies (2017)
27-ID (HEX): High Energy X-ray Diffraction (2020)

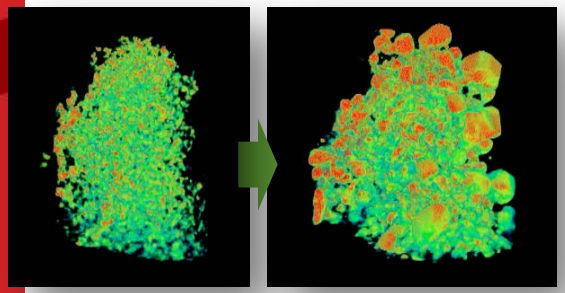
Motivation: Multi-dimensional x-ray imaging

Need 1

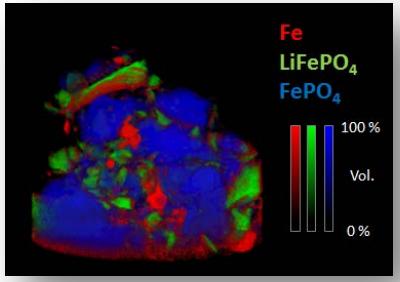
3 Dimensional (Spatial) Characterization



In situ 3D morphology evolution

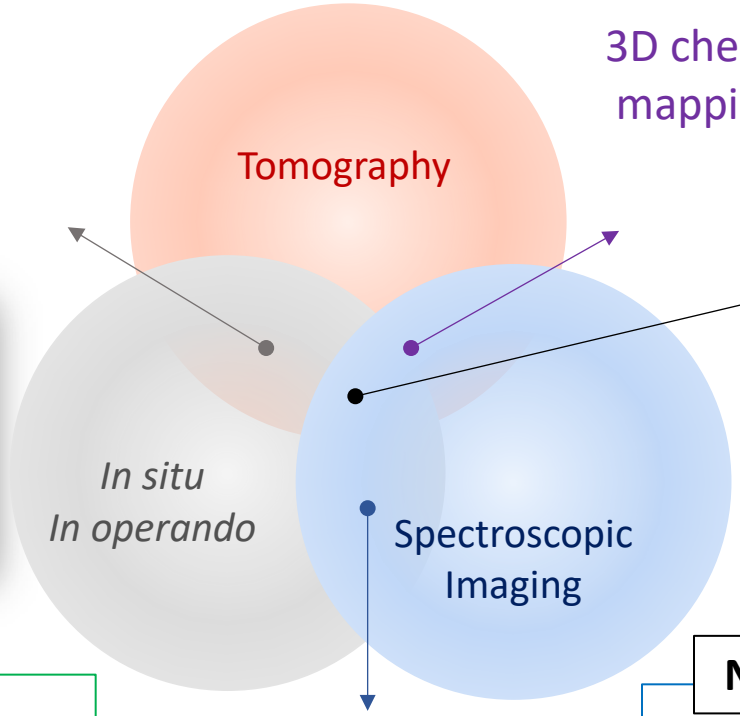


Solid oxide fuel cells

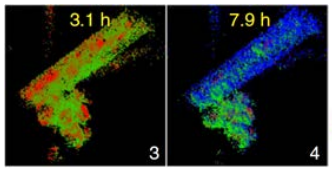


3D chemical mapping

Li-ion Battery



***In situ* 3D morphological Elemental/chemical Time-dependent evolution**



Li-ion Battery

Need 2

Time resolved with real Environment

In situ chemical evolution

Need 3

Elemental & Chemical sensitivity

Motivation: Multi-modal synchrotron approach

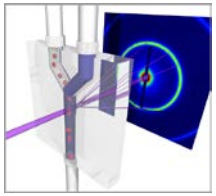
Suite of beamlines with complementary techniques - enabling time-resolved, *operando*, multi-modal and multi-dimensional studies

Scattering **Diffraction** **Spectroscopy** **Imaging**

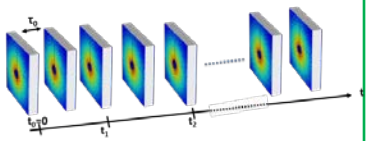
Structure

Chemistry

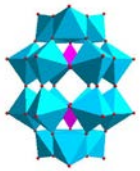
Morphology



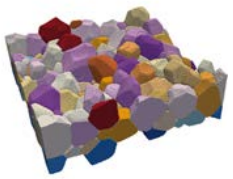
CMS



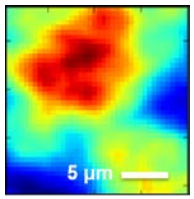
CHX



XPD



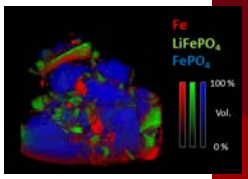
ISS



SRX

HXN

FXI



(XPD): X-ray Powder Diffraction

(ISS): Inner Shell Spectroscopy

(SRX): Sub-micron Resolution X-ray Spectroscopy

(CMS): Complex Materials Scattering

(HXN): Hard X-ray Nanoprobe

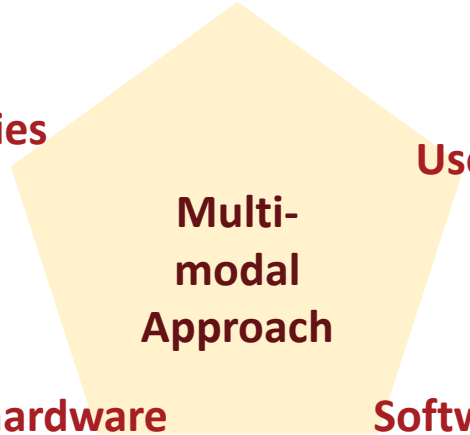
(CHX): Coherent Hard X-ray

(FXI): Full-Field X-ray Imaging

The Multi-Modal Issues Task Force @ NSLS-II

to identify the issues involved in **utilizing techniques across multiple beamlines** at NSLS-II, and in combining synchrotron techniques with **other techniques, such as the electron-based imaging methods at CFN**.

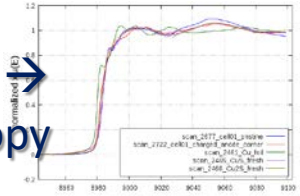
Potential research schemes and impact



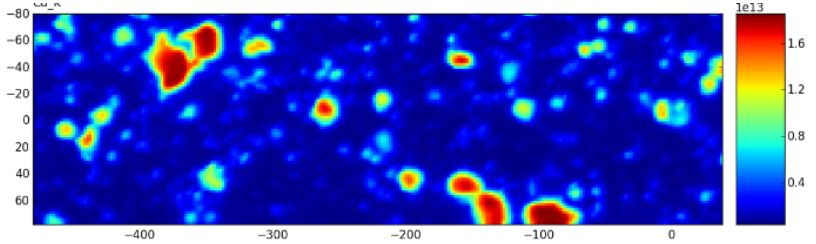
Morphology → imaging

Structure → diffraction & scattering

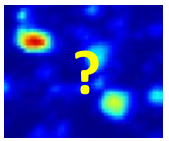
Chemistry → spectroscopy



Complex **Heterogeneous**

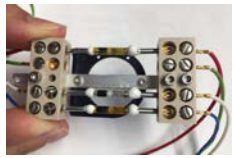


Li-S battery with CuS addtives



Particles (material)

Clusters (Electrodes)



Interfaces & Devices (System)

Themes

Theme I: Grand challenges on multi-dimensional and multi-modal imaging and analysis

Theme II: Improvement on multi-dimensional and multi-modal data collection and pre-processing

Theme III: Multi-modal contrast & length scale registration and correlation

Theme IV: Quantification, visualization and modeling in multi-dimensional and multi-modal imaging

Announcements:

- We will post all the workshop talks on the meeting website and link to the meeting summary - we will collect speakers slides during the workshop.
  - Two folders on the workshop computer: save vs delete
  - Save? Good to go; Delete? Please provide your reduced slides by today
- Lunch will be held at the workshop location.
- A photo session has been scheduled during the workshop (during afternoon break)
- Poster & Exhibition Session 5:30-7:30
- We will provide a workshop summary for publication/reporting purposes.

Themes

Theme I: grand challenges on multi-dimensional and multi-modal imaging and analysis

Section Chair: Lisa Miller

Stuart Campbell, Brookhaven National Laboratory
Grand Challenges of Multi-dimensional and Multi-modal Imaging and Analysis at NSLSII

Mark Basham, Diamond Light Source Ltd.
Multi-dimensional and Multi-modal Imaging and Analysis at the Diamond Light Source

Lisa Miller, Brookhaven National Laboratory
Discussions on Theme I

Theme I: grand challenges on multi-dimensional and multi-modal imaging and analysis

Session discussion lead: Lisa Miller

- **How do other facilities, companies, institutions visualize and analyze multi-modal (including imaging) data?** Are these data analyzed by separate tools and put together by a researcher's interpretation? Or are there tools that can facilitate this process by loading data from different contrast mechanisms and visualizing & analyzing them together? How do people do data management and keeping track, organizing different data sets?
- **There are already existing libraries and algorithms** which can be applied to multi-modal, multi-dimensional image analysis, e.g. image registration, multi-dimensional visualization. However these applications seem to remain as highly specialized fields, and tools aren't widely adopted by general users. **What are the true bottlenecks in this process?** Is it the implementation of the algorithms/libraries into user-friendly tools? Is it the education and outreach for people to learn about that those tools exist? Is it the training for researchers to become fluent in using those tools? Is it the communication between different fields (e.g. CS and the physical science)? And how do we overcome these barriers as a community (beamline/facility staff and user groups)?

Theme I: grand challenges on multi-dimensional and multi-modal imaging and analysis

Session discussion lead: Lisa Miller (con't)

- **What are the good strategies for physical science researchers (materials science, physics, chemistry, biology, geology, etc.) to partner with CS community (open source and companies) on conducting complex imaging analysis?** How do we balance between the needs of different parties - E.g. for a user facility, the main needs might be on implementation, and not on developing new algorithms or new computational architecture. However for CS groups (or computer scientists in a user facility), there is a need and motivation to develop new computational scientific methods, etc. How do we balance these two?

- **What is the vision on different modes of data processing - users process the data locally vs remotely?** What are the pros/cons and the trend that you observe at your facility or community? For multi-modal, multi-dimensional imaging analysis, is one better than the other?

Themes

Theme II: Improvement on multi-dimensional and multi-modal data collection and pre-processing

Section Chair: Yong Chu

Patrick La Riviere, University of Chicago
X-ray Fluorescence Computed Tomography: Novel Reconstruction Algorithms and Acquisition Strategies

Doga Gursoy, Argonne National Laboratory
Data Alignment in X-ray Nano-tomography

Yong Chu, Brookhaven National Laboratory
Discussions on Theme II

Theme II: Improvement on multi-dimensional and multi-modal data collection and pre-processing

Session discussion lead: Yong Chu

- **Tomography for scanning microscopy has additional complexity** than the full field counterpart:
  - Each image could be slightly distorted due to drift or other reasons.
  - Each image could contain scanning artifacts (i.e. streaks) due to beam instability.

It would be good to design an iterative tomography reconstruction taking into account of these errors. One thing that I can think of is: a) perform tomography reconstruction without the questionable images b) compare the projected image (i.e. calculated based on the reconstruction) with the acquired image. c) using a certain metrics for image quality, perform correction on the acquired image d) insert the corrected image and perform tomography reconstruction. Then, repeat a)-d) until the data converges.

Theme II: Improvement on multi-dimensional and multi-modal data collection and pre-processing

Session discussion lead: Yong Chu (con't)

- **Sparse to dense data collection.** For synchrotron applications, the 3D data are usually acquired "densely" (i.e. collect more data than needed). Thus, it would be good to integrate an approach for 3D reconstruction, starting with sparse data set and add more projections during the experiment. Would like to know if such data collection has been implemented at other facilities. If so, we should try to adapt the method.

Theme II: Improvement on multi-dimensional and multi-modal data collection and pre-processing

Session discussion lead: Yong Chu (con't)

- **"Smart" 3D data collection.** For nanoscale tomography, a limited circle of confusion for a rotary stage creates significant measurement trouble. Since it is not easy to predict where the center of the image would be before starting the measurement, scientists take one of the two approaches. One, use a large FOV and run automatic scan. This increase the total data collection time. Two, perform a coarse scan first. Then, center the sample and perform a high resolution image. This also adds time and additional radiation dose to the sample. It would be good to have a "smart" pattern recognition of an acquired image, so that the program can find out if the part of the image is missing or truncated (as a human can do). Then, shift the sample and collects only the "missing data". My emphasis is on a word "smart". We have tried "simplistic" approaches using centroid or object boundary. However, all of these failed. Unless a sample is isolated, 2D project images contain other objects (which you do not care) at particular angles. They come and go, depending on the angle. Algorithm should be "smart" enough to find out which is the part of the sample you care. Then, compute how much is "missing", so that only the "missing" portion can be measured. A human being has no trouble of doing this rather simple task but it is unclear if software can do the same work. I am sure it can but such software has not migrated into the beamlines yet. We should try to find out if we can take a similar method, used elsewhere.

Theme II: Improvement on multi-dimensional and multi-modal data collection and pre-processing

Session discussion lead: Yong Chu (con't)

- **Absorption correction for XRF tomography.** There is an urgent need for performing absorption correction for XRF tomography data set. Good to find out how the other facilities do on this problem and integrate the program at the NSLS-II.

Themes

Theme III: Multi-modal contrast & length scale registration and correlation

Section Chair: Stuart Campbell

Matthew McCormick, Kitware, Inc.
An Overview of Multi-dimensional, Multi-modal, Image Registration Methods and their Application with the Insight Toolkit (ITK) and Tomviz

Yijin Liu, Stanford Synchrotron Radiation Lightsource
Data Mining in Correlative Multi-modal X-ray Microscopy

Stuart Campbell, Brookhaven National Laboratory
Discussions on Theme III

Theme III: Multi-modal contrast & length scale registration and correlation

Session discussion lead: Stuart Campbell

- Different contrast mechanisms require different sample preparations, e.g. thickness limitations for µ-diffraction. What impact do such limitations have on the versatility of multi-modal imaging?
- Is it possible to correlate very different information per image pixel directly while taking an image so that the scientist can immediately judge the information content in his scan? This might require a significant amount of computing on the fly.
- Are tools available that can be given to users for further analysis of their data, for instance, XRF and XRD data? Who is teaching them how to use these tools, first one by one, second for an overlay of different data types?

Themes

Theme IV: Quantification, visualization and modeling in multi-dimensional and multi-modal imaging

Section Chair: Thomas Caswell

Mike Marsh, Object Research Systems, Inc.
Easy Integrated Analysis and Visualization of Multi-modal and Multi-dimensional Image and Spectral Data with Dragonfly

Daniela Ushizima, Lawrence Berkeley National Laboratory
High Throughput Reverse Image Search with pyCBIR: Quantification, Search, Retrieval and Ranking for Multi-modal Imaging

Thomas Caswell, Brookhaven National Laboratory
Discussions on Theme IV

Theme IV: Quantification, visualization and modeling in multi-dimensional and multi-modal imaging

Session discussion lead: Thomas Caswell

- How do display high (non-spatial) dimensional data?
- How to display feature marks?
- How to display multi-scale images for alignment?
- How to track parallel coordinate systems?
- What tools do people use for image registration and alignment ?

Conclusion Remark & Summary from Discussions

Karen Chen-Wiegart

Theme I: grand challenges on multi-dimensional and multi-modal imaging and analysis

Theme II: Improvement on multi-dimensional and multi-modal data collection and pre-processing

Theme III: Multi-modal contrast & length scale registration and correlation

Theme IV: Quantification, visualization and modeling in multi-dimensional and multi-modal imaging

Thanks you!
Please attend the poster and exhibition session
5:30-7:30 pm

A casual gathering

- **Time: starting at 8 pm**
- **Location: BBD's - Beers Burgers Desserts (49 NY-25A, Rocky Point, NY 11778)**