User and CAT Issues

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APSUO/PUC Meeting

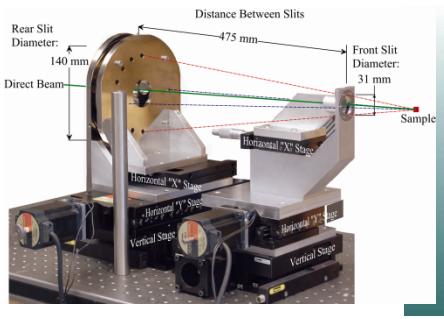
January 28, 2015

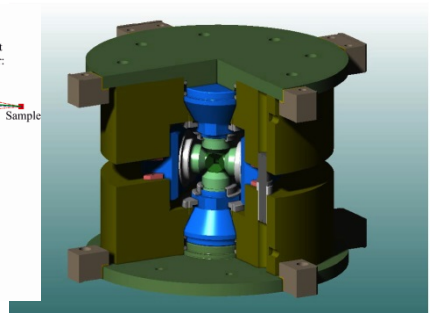
Agenda

- Update on NSLS II Transition Activities (6-BM, 8-BM, 13-BM)
- Proposed new year-end reporting process for CATs
- Summary of short-term BL improvement plans submitted by CATs
- Conversation with one of the CATs

6-BM: White Beam Energy Dispersive Diffraction

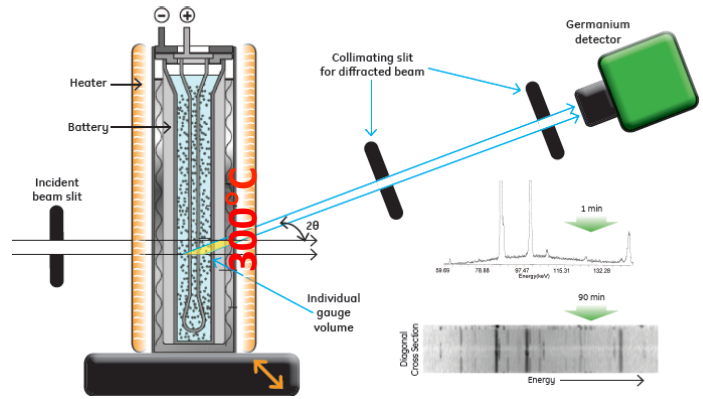
6-BM-B: High Pressure EDD





COMPRES – High pressure Earth sciences consortium

6-BM-A: General EDD



GE Global Research, Rutgers University, BNL, Engineering/Battery research

HP-EDD (~50%)

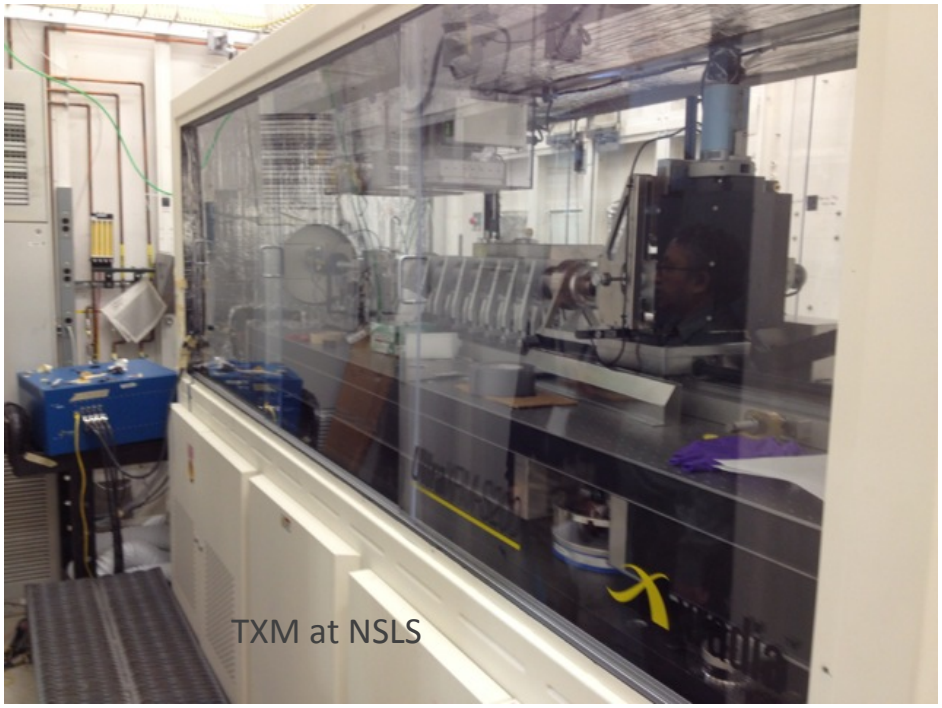
- Supported by COMPRES (Stony Brook U.)
- Large volume press being shipped to APS week of Feb. 2 (3 SB staff will come to assist in installation)
- Stony Brook staff (Hainyan Chen) to relocate to Chicago

General – EDD (~50%)

- NSLS equipment (detectors, stages, charging cell) expected shipping week of Jan. 26
- NSLS staff (Zhong Zhong) will come early Feb. to assist with setup

"A few" General Users expected for late 2015-1; full GU operation to start 2015-2

8-BM: NSLS Transmission X-ray Microscope



8-BM

- MOU for TXM at 8-BM signed.
- GU beamtime allocation will be approximately half for TXM and half for hard x-ray micro-fluorescence (existing program on 8-BM).
- BNL will support the TXM users and APS will support micro-fluorescence users.
- Initial flux calculations indicate possible decrease in performance relative to operation at NSLS.

- NSLS has already contacted Xradia and current plan is to have TXM crated in by January 30, 2015.
- The TMX is likely to be be installed at the end of 2015-1 run cycle.
- Commissioning/Friendly users in 2015-2 cycle with general user operations in the 2015-3 cycle.

13-BM-C: Diamond Anvil Cell Activities with COMPRES

- To accommodate monochromatic DAC work, a Si 311 single-bounce monochromator crystal has been commissioned, ~30 keV fixed energy.
- 300 mm long horizontal focusing mirror bender has been ordered from IDT. Mirror has been ordered from Coastline Optics.
  - Delivery of mirror and bender expected in early February
  - Mirror box is complete, and a 200 mm long mirror is being used temporarily for commissioning
- A new optical system for viewing, laser-heating and spectroscopy (Raman, ruby fluorescence, and temperature measurement) has been designed. Phase 1 of this system has been fabricated and is being used for commissioning.
- The COMPRES COMPTECH hire, Jin Zhang, started in the beginning of November. She is participating in the 13-BM-C commissioning.
- The COMPRES PX2 hire, Dongzhou Zhong, whose primary responsibility will be 13-BM-C, started at the beginning of January.
- Commissioning experiments are in progress, and will continue with first "friendly users" in 2015-1. We expect to make the system available to the GU system in 2015-2.

Assessing CAT Financial Health on an Annual Basis

- During discussion of Beamline Review Reports at the last SAC meeting (Nov 2014), several members pointed out that the APS does not always have up-to-date information of the financial status of the CATs.

- Although each CAT reports its sector funding at the end of the fiscal year to the APS for inclusion in the BES Annual Facilities Questionnaire, APS management only gets a reasonably close look into the funding situation once every 5 years.

- Recommendation from the SAC:
  - *In light of financial difficulties uncovered in some recent reviews, the SAC recommends that APS management work with the Partner User Council to create a mechanism to assess CAT financial health on an annual basis*.

- We propose to develop a one page financial questionnaire that is filled out by the CATs at the end of the fiscal year.
  - Funding level for previous FY
  - Expected funding level for next FY
  - If significantly different, provide short explanation
  - Expiration date of current funding grant/proposal/agreement/etc.

CAT Beamline Improvement Plans

- I've been gathering information from the CATs about how their plans for beamline improvements/enhancements, both short-term (1-3 yrs) and long-term (>3 yrs).
  - recent SAC Beamline Reviews
  - e-mail requests

- I also tried to collect some information on how the longer-term enhancements that would be needed to utilize a near-diffraction limited beam.

- Thought it might be interesting to share some of the information I collected with the APSUO and PUC members.

- This is a summary of the current information I have on the **short-term improvements** that the CATs have in mind.

- If I missed something, plans have changed or you would like to add something, please let me know and I will do so and post the updated version.

CAT PX Beamline Improvement Plans

SER CAT

- Doubling of 22-ID's robotic sample handling capacity
- Continue activities with extended wavelength crystallography

GM/CA

- Enhance micro-crystallography capability with a new micro-focus endstation, now in development on beamline 23-ID-D.
- Increase use of energies at 7 keV with longest-possible helium path to the detector and a beam stop that minimizes scatter from the primary beam.
- New PAD detector

NE CAT

- Reconfigure the E-line (fixed-energy) single crystal side-bounce monochromator.
- During the spring shutdown install a secondary compact Kirk-Patrick Baez focusing system on the E-line to take the focus spot size from its current 15 x 100 microns (v x h) to something approaching 5 x 5 microns.
- On the C-line, replace the VFM with one with a surface error in the range of 0.2 – 0.4 micro-radians for better ability to give an unstructured beam during under- and over-focused conditions.

CAT non-PX Beamline Improvement Plans

DND CAT

- On 5-ID
  - Install compound refractive lenses for smaller beams for both surface diffraction and SAXS.
  - Improve stability from our current monochromator and mirrors, which will only be of concern once the new detector system is running at 100 frames per second routinely.
  - Increase the high-energy limit from 17 keV to 25 keV by reducing the vertical offset of the high heat load monochromator.
- Install a toroidal mirror for horizontal focusing on 5-BM.

MR CAT

- Replace the current monochromator with an improved design (on-going).
- Improve the microbeam spectroscopy facility adding x-ray emission analysis.
- Add a totally new capability: High-energy x-ray photoemission.

GSE CARS

- Anew program for single-crystal diffraction with laser heating in the DAC for 13-BM.
- Further develop the D-DIA apparatus for deformation experiments at high pressure in the multi-anvil press.
- Upgrade the microprobe apparatus to advance ease of experiment set-up for low-energy measurements.

CAT non-PX Beamline Improvement Plans (cont)

ChemMat CARS

- Install a second crystallography diffractometer optimized for high pressure charge density and *in-situ* high energy diffraction under extreme conditions.
- Procure a PILATUS3 1M PAD for crystallography.
- Install compound refractive lenses (CRL) to optimize focusing of high energy x-rays.
- Develop high energy x-ray techniques for liquid surface scattering that will enable large Q measurements of liquid surface structure.

Bio-CAT

- Improve detectors for time-resolved studies.
- Fiber micro-diffraction at small and wide angles.
- Efficient, high throughput, combined SAXS and liquid chromatography.
- Advanced microfluidic mixers with microbeams for continuous flow, sub millisecond time resolution micro-beam SAXS.
- ms-time resolved kinetic SAXS with dramatically lower sample consumption.

Nanoprobe

- Upgrade the capability for *in-situ* temperature and electric/magnetic field manipulation, and implementation of a diamond phase retarder for generation of polarized x-rays for nano-magnetism experiments.

Recent Discussions with APS CATs

- One of the CATs said they would contribute a person's time to develop beamline software as part of a coop of sorts where the finalized software is available to the whole group. A possible solution for the software developer shortage.

  Would CATs consider contributing staff time and how much and if there is enough interest create a consortium managed by AES?

- While it is too expensive for the detector pool to purchase everything the beam lines want, CATs could pay a percentage of the cost of a detector in return for getting to use if for that same percentage amount of time.

  Would CATs be interested in such an arrangement?

- To keep work in-house during the APS upgrade installation period, CATs could consider using available staff from other CATs rather than hiring out-side workers for some BI improvements.

  Would CATs be interested in such an arrangement?

EXTRA SLIDES WITH MORE DETAILED CAT SHORT TERM BL IMPROVEMENTS

DND CAT

DND CAT

- We plan to continue to invest heavily in our SAXS/MAXS/WAXS capability on the ID line and the XANES/EXAFS capabilities on the BM line.
  - On 5-ID, we plan to implement compound refractive lenses to enable moderate improvements in the flux on sample and to allow us to create smaller beams for both surface diffraction and SAXS.
  - We also plan to diagnose and correct a few minor beam instabilities from our current monochromator and mirrors, which will only be of concern once the new SAXS/MAXS/WAXS detector system is running at 100 frames per second routinely.
  - We also plan to increase the high-energy limit from 17 keV to 25 keV by reducing the vertical offset of the high heat load monochromator.

  - On 5-BM, we plan to install a toroidal mirror for horizontal focusing.

- We already have expertise in absorption-based x-ray microtomography, and thus plan to explore the possibility of doing sub-micron resolution tomography of low-absorption-contrast samples

MR CAT & GSE CARS

MR CAT

- Replace the current monochromator with an improved design (on-going).
- Improve the microbeam spectroscopy facility and (taking advantage of the better focusing) add x-ray emission analysis.
- Work with the APS to allow variable speed undulator scanning to match quick-scan monochromator.
- Add a totally new capability: High-energy x-ray photoemission.

GSE CARS

- Bring the 13-BM-C station fully online with additional scientific programs in interface diffraction and new programs in diffraction at high pressure; this will include a single-crystal diffraction with laser heating in the diamond anvil cell.
- Further develop the D-DIA apparatus for deformation experiments at high pressure in the multi-anvil press.
- Further develop the high-pressure tomography technique in the multi-anvil press.
- Develop high-speed pink-beam microtomography for time-resolved studies of fluid flow
- Upgrade the microprobe apparatus to advance ease of experiment set-up for low-energy measurements.

BioCARS & ChemMat CARS

BioCARS

- Conduct a one-day "brainstorming session" in November to explore future scientific avenues for BioCARS with a number of external experts.
- Continue to develop ties to other, largely APS-based sectors with a strong interest in dynamics.

ChemMat CARS

- Our main goals during the next three years are:
  - install a second crystallography diffractometer optimized for certain state of the art techniques, such as high pressure charge density and *in-situ* high energy diffraction under extreme conditions
  - obtain a PILATUS3 1M PAD for crystallography, which will provide much faster response, dynamic range, Q-range, and energy range than our current Bruker APEXII
  - install compound refractive lenses (CRL) to optimize focusing of high-energy x-rays
  - development of high energy x-ray techniques for liquid surface scattering that will enable large Q measurements of liquid surface structure.

HP CAT, IMCA CAT, & Bio-CAT

HP CAT

- No short-term info available - focus was on upgrades for MBA

IMCA CAT

- No short-term info available - longer term would like canted IDs

Bio-CAT

- Time and Spatially-Resolved Fiber Diffraction
  - Improved detectors and beamline enhancements for time resolved
  - Fiber micro-diffraction at small and wide angles
  - Coordinated Micro-diffraction imaging and X-ray Fluorescence Microscopy
- High performance static SAXS for challenging studies of macromolecules and their complexes
  - Efficient, high throughput, combined SAXS and liquid chromatography
  - Improved Q-range to access larger structures at higher resolution
- Time-resolved SAXS
  - Advanced microfluidic mixers with microbeams for continuous flow, sub-millisecond time resolution micro-beam SAXS
  - ms-time resolved kinetic SAXS with dramatically lower sample consumption
  - Pump-probe capability for 500 ns time resolution

SBC CAT, LS CAT, SER CAT & GM/CA

SBC CAT

- No short-term info available - focus was on upgrades for MBA

LS CAT

- No short-term info available - focus was on upgrades for MBA

SER CAT

- Planned doubling of 22-ID's robotic sample handling capacity
- Continue activities with extended wavelength crystallography

GM/CA

- Further enhance the micro-crystallography capability with a new micro-focus endstation, now in development on beamline 23-ID-D.
  - use the existing Kirkpatrick-Baez (KB) mirrors to image the undulator source to a position upstream of the endstation, creating a secondary source. A set of micro-focusing KB mirrors would image the secondary source to the sample position.
- Increase use of energies at 7 keV or lower by optimizing a prototype of the micro-focus endstation to include a longest possible helium path to the detector and a beam stop that minimizes scatter from the primary beam.
- New PAD detector

NE CAT, Nanoprobe & LRL

NE CAT

- Reconfigure the E-line (fixed-energy) single crystal side-bounce monochromator for improved beam position and thermal stability.
- During the spring shutdown, we will install a secondary compact Kirk-Patrick Baez focusing system on the E-line to take the focus spot size from its current 15x100 micron (VxH) to something approaching 5 x 5 micron.
  - The secondary KB system is from IDT, already on hand…just awaiting delivery of the support structure for it (ADC), to be delivered in spring 2015. These mirror have been through APS metrology and look pretty good.
- On the C-line, replace the VFM with one with a surface error in the range of 0.2 – 0.4 micro-radians and better ability to give an unstructured beam during under- and over-focused conditions. This mirror will be contracted in fiscal 2015.

Nanoprobe

- Upgrades including the capability for *in-situ* temperature and electric/magnetic field manipulation, and implementation of a diamond phase retarder for generation of polarized x-rays for nano-magnetism experiments.

LRL CAT

- No short-term info available