

... for a brighter future

# APS Renewal Instrumentation Part I

Denis Keane, Director DND-CAT, PUC Chair Scientific Advisory Committee (SAC) Meeting January 20-22, 2009



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### Areas Covered in Part I

#### Introduction

#### Instrument Groups

- Crystallography
- Bulk Probes
- Spectroscopy
- Surface Probes



### Introduction

#### Today's presentations

Renewal Steering Committee

- Denny Mills, PSC, Chair Techniques II
- Denis Keane, PUC (DND) Techniques I
- Paul Fuoss, APSUO (MSD) Integration with Science Cases
- Other Members: Rod Gerig, PSC; George Srajer, XSD; Bob Fischetti, PUC/LSC (GM/CA); John McLean, AES; Dan Neumann, SAC (NIST)

#### Basis

- Instrument Groups
  - Beamline Proposals
  - LOIs, CAT/CDT Proposals
  - Open Forum of January 9, 2009
  - Committee members
- Science Drivers & Integration
  - All of the above
  - Science Cases
  - Renewal Workshop of October, 2008



### Introduction II

- Comments
  - Several CATs provide multiple techniques and will continue to do so, based on funding and APS reviews
    - GSE-CARS
    - ChemMat-CARS
    - HP-CAT
    - DND-CAT
  - Difficult to account for distributed capabilities in some cases
  - Can miss synergies when categorizing by technique (SAXS/WAXS/PDF on one beamline?)

#### Definition

- Beamline
  - Operates independently of others
  - May have dedicated or shared source
  - Has dedicated shutter
- Station
  - Enclosure for experiments
  - One beamline can have several stations



### Macromolecular Crystallography

Some Comments

- APS leads the world in PDB deposits
- Around 40% of APS users are MX researchers
- All MX beamlines are CATs (non-XOR)
- Four sectors are "new": SER, GM/CA, NE, LS (last 3 canted IDs)
- One rebuilt/new sector has been discussed with 1 micron beams (not currently in list of LOIs but LSC is considering again)
- Summary of Beamline Renewal Proposals and Sector LOIs/Proposals
  - Emphasis on advanced detector technology
    - Proposal for APS support of anticipated PAD detectors
  - Additional key needs are in small beams
    - New focusing optics
    - Beam stability especially angular stability
    - Beamline stability





### **MX Beamlines**

Existing BL Operator (% currently)	Upgrade Proposal or LOI/New Proposal (% future)	Techniques and Disciplines	Beam Properties/ Unique?
14IDB, 14BMC BioCARS (2)	14ID rebuild 2008 (2)	BSL3, Laue crystallography (also in time resolved	UNIQUE
17IDB, 17BMB IMCA (CARS) (2)	17ID rebuild 2008 (2)	Industrial collaboration, MAD/SAD	
19IDD, 19BMD SBC (2)	Upgrade/move(?) including 1 micron beams (3)	MAD/SAD, Ultralow temperature (15K)	1 μm UNIQUE
21IDD, 21IDF, 21IDG LS-CAT (3)	Complete side bounce station 21IDE – ongoing now (4) – 2 canted undulators	MAD/SAD	200-100 μm
22IDD, 22BMD SER-CAT (2)	(2)	MAD/SAD	200-100 μm
23IDB, 23IDD GM/CA-CAT (2)	(2) – 2 canted undulators	MAD/SAD, microbeams	200-5 μm
24IDC,24IDE NE-CAT (2)	(4) – 2 canted undulators, complete 24BM, add final ID station	MAD/SAD, microbeams	200-20 μm
31ID SGX (1)	(1)	SAD	
<b>16.0</b> (equivalent)	<b>20.0</b> (equivalent)	Canted and Tandem IDs no new BLs	



### **Powder Diffraction and Crystallography Instruments**

- Some Comments
  - Powder Diffraction is an integral part of <u>Real Materials in Real</u> <u>Conditions</u> but can it be made into <u>Real Time?</u>
  - Part of a continuum of reciprocal space techniques complementary to imaging: single crystal, powder, WAXS, PDF, EXAFS, SAXS
  - One of many techniques for High Pressure research on HP-CAT





### **Powder Diffraction and Crystallography Beamlines**

Existing BL Operator (% currently)	Upgrade Proposal or LOI/New Proposal (% future)	Techniques and Disciplines	Beam Properties/ Unique?
5BMC DND-CAT (50%)	Add focusing (50%)	Chemistry, Materials Science, tunable	
5IDB DND-CAT (25%)	Increase access through upgrade to 2 canted undulators (50%)	11-detector system could be upgraded to 11BM style for ultimate resolution	UNIQUE to APS
11BM XOR (100%)	(100%)	Improved multi-detector system	UNIQUE to APS
	New high-resolution 2-d detector based system (100%)	Materials Science	
13BMC GSE CARS(25%)	(25%)	Single Crystal Diffraction, Geology, Environmental Science	
15IDC ChemMatCARS (33%)	Upgraded optics (33%)	Single Crystal Diffraction, Materials Science, chemistry	
16IDB, 16IDD,16BMB, 16BMD HPCAT (3.5)	Specialized IDs, canted IDs (4)	Powder diffraction, single crystal diffraction; High pressure, Geology, materials science	
<b>5.8</b> (equivalent)	7.6 (equivalent)	New instrument for new beamline, canted IDs	



#### **Bulk Probes**

- Some Comments
  - Includes PDF, SAXS, diffraction and diffraction imaging
  - APS is world competitive in (at least) several areas:
    - Dedicated PDF beamline
    - White beam Laue micro-diffraction
    - High Energy diffraction microscopy
  - Detector technology (i.e. GE angio) key to current and future capabilities





## High Energy Beamlines

Existing BL Operator (% current)	Upgrade Proposal or LOI/New Proposal (% future)	Techniques and Disciplines	Beam Properties/ Unique?
1-ID XOR (100%)	Improved optics and detectors dedicated to part of existing 1ID program SCU (100%)	High energy studies of aggregate polycrystalline materials Materials science, engineering	~ μm spatial resol. 40-90 keV
	New beamline for HEDM ,SCU (100%)	Materials science, Hierarchical Imaging	~ μm spatial resol. 40-90keV
	New BM beamline for HE studies (100%)	Energy Dispersive Diffraction, High E tomography, Materials science	~ μm spatial resol.
11-ID-B XOR (50%)	Optimized ID. Dedicated for PDF (100%)	Materials science, chemistry	UNIQUE
11-ID-C XOR (50%)	Improved optics and detectors (100%)	High Energy Diffraction, PDF, materials science, chemistry	~ μm spatial resol
	New beamline for submicrofocus HE (100%)	High Pressure, Materials science	~ 200 nm spatial
6IDD XOR (50%)	(50%)	PDF, High E diffraction, Mat Sci	
13ID GSE (25%)	Canted ID (50%)	Geology, Environmental Science	
5BMD DND (25%)	Upgrade Monochromator (25%)	Materials Science, Chemistry	
<b>3.0</b> (equivalent)	<b>7.25</b> (equivalent)	Canted and Optimized IDs and one new BM BL	



### SAXS beamlines

Existing BL Operator (% current)	Upgrade Proposal or LOI/New Proposal (% future)	Techniques and Disciplines	Beam Properties/ Unique?
1ID XOR (25%)	New dedicated beamline, SCU (100%)	HE SAXS/WAXS Materials science	
5IDD DND (50%)	Canted ID (100%)	SAXS/WAXS; polymers, nanoscience Materials science, chemistry	Doubly focused, 50 µm beam
8ID XOR (50%)	Optimize and dedicate station to GISAXS (50%)	GISAXS, polymers, materials science, chemistry	
12ID XOR (50%)	Canted ID upgrade underway (150%)	SAXS/WAXS/GISAXS/USAXS, chemistry, materials science	
15ID ChemMat CARS (33%)	Upgrade optics (33%)	SAXS, Chemistry, Materials Science	
18ID BioCAT (50%)	Tandem undulators to increase flux (50%)	Solution Scattering	Double focused ID
32ID XOR (25%)	To 12ID(?)	USAXS	
<b>2.8</b> (equivalent)	<b>4.8</b> (equivalent)	Canted IDs and one new ID BL	



## Laue Diffraction Microscopy

Existing BL Operator (% current)	Upgrade Proposal or LOI/New Proposal (% future)	Techniques and Disciplines	Beam Properties/ Unique?
34ID XOR (50%)	Triple Canted IDs, nanoprobe (200%)	3D microscopy, materials science, engineering	300 nm & 50 nm UNIQUE
0.5	2	Canted ID, new station	

#### Magnetic Scattering (non-resonant)

Existing BL Operator (% current)	Upgrade Proposal or LOI/New Proposal (% future)	Techniques and Disciplines	Beam Properties/ Unique?
4IDD XOR (50%)	New ID, improved optics (50%)	XMCD, diffraction, physics, materials science	
6ID XOR (50%)	(50%)	diffraction	
11IDD XOR (50%)	(50%)	diffraction	
	New beamline (100%)	15T superconducting magnet, pulsed magnet, future high- field magnet outfield station	>30 keV, 100 µm x 100 µm
2	3	New beamline	



### Spectroscopy and the APS Renewal

- Bulk XAS
  - Many BM beamlines currently support the technique: 5BMD, 9BM, 12BMB,13BMD,20BM; 10BM soon to be online
  - 9BM already scheduled for upgrade/renewal with LDRD for catalysis
  - Effort during renewal should be overall coordination of efforts especially in improving detectors, sample environments and software
- Need for dispersive EXAFS on ID line at APS?
- Microprobe based XAS
  - APS may be lagging in K-B based systems several upgrades are proposed
  - Critical need for sample environments is cryogenic sample preservation



### Nano/Micro XAS

Existing BL Operator (% current)	Upgrade Proposal or LOI/New Proposal (% future)	Techniques and Disciplines	Beam Properties/ Unique?
2-ID XOR (33%)	Cryo-XRF beamline (100%) + room temperature microprobe (50%)	Biology	500 nm - 30 nm
	BioNanoProbe (50%)	Biology	~30 nm
13-ID GSECARS (50%)	Canted ID with improved KB focusing (100%)	Geology, Environmental Science	Scan large area, zoom in w/ sub-µm beam
16ID HP-CAT (50%)	Canted ID with improved KB focusing (100%)	High Pressure Science	sub-µm beam
18ID BioCAT (50%)	Dual inline undulators to improve flux , new optics (50%)	Biology	
20ID XOR (50%)	Canted ID with improved KB focusing (100%)	Environmental Science, Materials Science	Scan large area, zoom in w/ sub-µm beam
26ID XOR/CNM (50%)	(50%)	Materials Science, Nanoscience	Better than 30 nm resolution, UNIQUE
<b>3.8</b> (equivalent)	<b>6.0</b> (equivalent)	Canted IDs and one new ID BL	



#### **Time Resolved EXAFS**

Existing BL Operator (% current)	Upgrade Proposal or LOI/New Proposal (% future)	Techniques and Disciplines	Beam Properties/ Unique?
7IDD XOR (50%)	improved focusing optics, HR emission spectroscopy (50%)	Laser pump-probe	Sub-ns resolution Psec pulse (?)
11IDD XOR (50%)	New ID, improved optics (50%)	Laser pump-probe	Sub-ns resolution
20IDD XOR (50%)	Canted ID, Detector and focusing upgrade (100%)	diffraction	Sub-ns resolution
1.5	2.0	1 canted ID	





Existing BL Operator (% current)	Upgrade Proposal or LOI/New Proposal (% future)	Techniques and Disciplines	Beam Properties/ Unique?
4IDC XOR (50%)	improved optics (50%)	Soft x-ray XMCD, PEEM, physics, materials science	
4IDD XOR (50%)	New ID, improved optics (50%)	XMCD, diffraction, physics, materials science	
	Low x-ray energy XMCD New beamline dual undulators (100%)	XMCD, physics, materials science	
1	2	New beamline	



### Inelastic X-ray Scattering

- Common needs
  - Improving the source
    - Long straight sections
    - Multiple optimized IDs superconducting, in-vacuum
    - Higher electron current in APS storage ring
  - Advancing detectors
    - Ge-based strip detectors with ~100 crystal analyzers
    - Improved APD arrays for NRS
  - Proposing 2 new spectrometers
    - Multi-Analyzer Spectrometer with > 100 Analyzer/Detector Assemblies
    - Ultra-High Resolution Spectrometer
      - 100 µeV
      - Using comb crystals





Existing BL Operator (% current)	Upgrade Proposal or LOI/New Proposal (% future)	Techniques and Disciplines	Beam Properties/ Unique?
3ID XOR (100%)	Source, new detectors (100%)	NRS, physics	0.5 meV and better
9ID XOR (50%)	Source, new focusing, new spectrometer, canted ID (100%)	Medium Resolution IXS	40-100 meV
16ID HP (25%)	Canted IDs (50%)	NRS, high pressure science	
20ID XOR (25%)	Canted IDs (50%)	LERIX, Materials Science	0.5-1eV
30ID XOR (100%)	Source, new detectors, new spectrometer (100%)	MERIX and HERIX, physics	To 100 μeV
<b>3</b> (equivalent)	<b>4.0</b> (equivalent)	New IDs, canted IDs	



#### **Surface Probes**

- Covers many techniques:
  - GISAXS
  - Surface & Interface Diffraction/Scattering, including resonant scattering, XSW, reflectivity
  - Liquid Surface Scattering
  - XAFS
  - In-situ capabilities
    - Especially can benefit from dedicated station
  - Some centralized, some distributed
- New applications
  - X-ray Interface Microscopy
    - See surface steps
    - Can upgrade/compliment many existing surface/interface experiments





## Surface Scattering (XSW, reflectivity, COBRA, etc.)

Existing BL Operator (% current)	Upgrade Proposal or LOI/New Proposal (% future)	Techniques and Disciplines	Beam Properties/ Unique?
	XIS proposal, canted IDs, side bounce mono, BM (5)	XSW, XRIM. Surface science	4-40keV, 10 keV,10keV ,30 keV
5ID DND (25%)	Canted ID, side-bounce mono (50%)	XSW, UHV chamber	
6ID XOR (33%)	Upgraded optics (33%)	UHV chamber	
12ID XOR (50%)	Canted ID, side bounce mono (50%)	MOCVD chamber, diffractometer	4.5-36keV
13ID GSE CARS (25%)	Canted ID, mirror offset (50%)	High energy interface diffraction/scattering – Mineral/water interface	5-100 keV
20ID XOR (25%)	Canted ID (33%)	MBE chambers, surface XAFS	
33ID, BM XOR (2)	Canted ID, side bounce mono, new larger station (3)	XSW, PLD	
<b>3.6</b> (equivalent)	<b>10.2</b> (equivalent)	New sector, canted IDs	



### **GISAXS**

Existing BL Operator (% current)	Upgrade Proposal or LOI/New Proposal (% future)	Techniques and Disciplines	Beam Properties/ Unique?
8-ID XOR (50%)	2 tandem undulators, new offset mono, new detectors (100%)	Polymer science, Materials science, chemistry	
12-ID XOR (25%)	Canted undulators, SAXS on 1.5 beamlines (75%)	Materials science, chemistry	
<b>0.75</b> (equivalent)	<b>1.75</b> (equivalent)	New ID, canted ID	



## Liquid Surface Scattering

Existing BL Operator (% current)	Upgrade Proposal or LOI/New Proposal (% future)	Techniques and Disciplines	Beam Properties/ Unique?
6ID XOR (25%)	(25%)	Soft condensed matter	
9ID XOR (50%)	Canted ID, side-bounce mono (100%)	Soft condensed matter	
15ID ChemMat CARS (33%)	Upgraded optics (33%)	Soft condensed matter, Materials Science, Chemistry	
<b>1.1</b> (equivalent)	<b>1.6</b> (equivalent)	Canted ID	



### **Summary/Discussion Points**

- Major capacity increases in
  - Surface scattering
  - High energy instruments
- Key optics improvements
  - New K-B mirrors for XAS micro/nano probes
  - Many side-bounce monochromators for canted ID beamlines
- Significant new instruments
- Development projects
  - High resolution 2-d powder diffraction
  - APS source stability improvements benefits all
- Detector needs
  - Pixel Array detectors for MX, SAXS
  - Fast spectroscopy (Si drift) for XAS
  - Ge strip detectors for IXS
  - APD arrays for NRS

