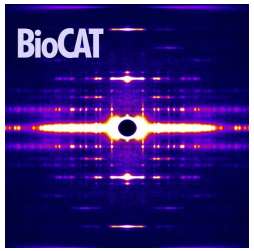

Benefits of APS-U and other planned developments on the BioCAT SAXS program

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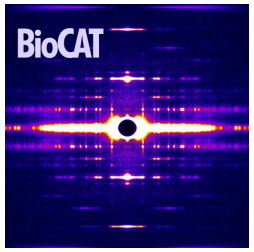
CSRRI



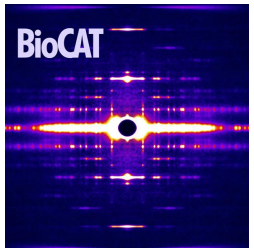
APS-U by the numbers

- Overall:
  - 3x increase in flux, to ~5*10^{13} ph/s
  - 8x increase in flux density
  - More symmetric beam with reduced horizontal size

- Equilibrium SAXS:
  - 6x increase in flux
  - 6x increase in flux density

- Time resolved SAXS:
  - 5-10x increase in flux
  - ~25x increase in flux density
  - More symmetric microbeam, 4x4 μm^2

	Flux (ph/s)	Beam size (μm^2)	Microbeam flux (ph/s)	Microbeam size (μm^2)
Now	1.5e13	30 x 140	2e12	4 x 20
APS-U	5e13	30 x 30	1e13	4 x 4

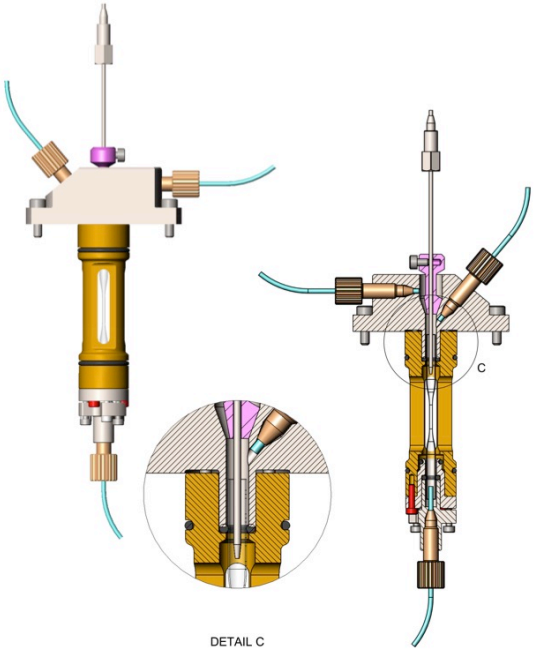


APS-U Benefits

- For all experiments:
  - Greater total flux and flux density will yield better signal to noise
  - Improved beam stability for more reliable baselines
- For equilibrium SAXS:
  - Reduced beam size in the horizontal should allow smaller beam stops, lower minimum q
- For TR-SAXS:
  - Smaller beam will allow earlier first time points
  - Improved signal to noise will allow reduction in sample consumption

APS-U Challenges

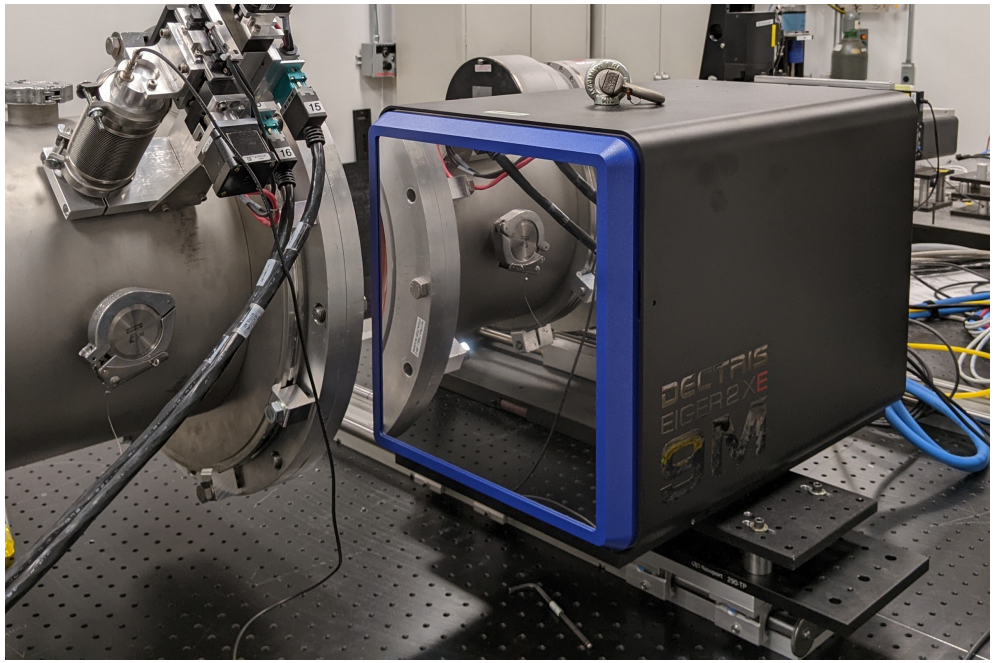
- Radiation damage
  - Increased flux density means a greater chance at radiation damage to samples
- For equilibrium SAXS, existing coflow sample cell should prevent radiation damage in most cases
  - The coflow geometry has been shown to be effective at preventing damage with up to ~10x greater flux than we will have post APS-U (Nigel Kirby, private communication)
  - Certain buffers are more prone to damage, addition of radical scavengers such as glycerol can be used to mitigate
- For TR-SAXS, may see significant damage with full beam
  - Can mitigate with faster scanning/flow
  - Addition of radical scavengers necessary
  - Possible re-design of mixers to include a sheath flow similar to the coflow cell (e.g. Pollack & Doniach, 2009)



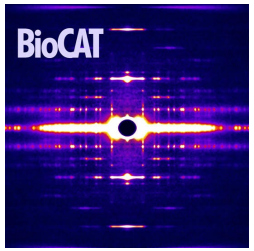
SAXS coflow sample cell

Recent SAXS improvements

- Eiger2 XE 9M detector
  - Larger area gives wider q range (currently q~0.42, planned q~0.5 1/A)
  - Smaller pixels given improved sampling in the low q (e.g. Guinier) region
  - Continuing high reliability
- Smaller beam stop
  - Minimum q improved from ~0.0045 to ~0.003 1/A

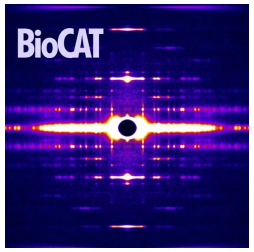


- Automated processing pipeline
  - Data reduced on the fly, initial analysis results (through bead models) available within ~5 minutes of end of experiment
  - Users no longer need to work with images, reducing overall data storage and transfer needs



Recent SAXS improvements

- Temperature control from ~5-50 C for SEC-SAXS and SEC-MALS-SAXS
- Availability of Ion-Exchange chromatography coupled SAXS (IEC-SAXS) and routine analysis for IEC-SAXS
- Routine deployment of laminar flow mixer for TR-SAXS
  - Time ranges from ~1 ms to 1.5 s, very low sample consumption
- Improved control software and scanning hardware for TR-SAXS, allowing for simple and reliable operation of all experiments
- Upgraded fluid delivery systems for TR-SAXS, to improve ease of operations and efficiency

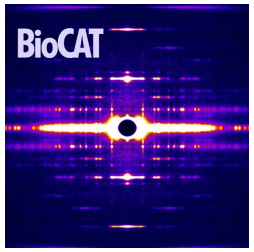


Planned upgrades

- APS-U dark period gives us time to do some major upgrades that might otherwise take away from user experimental time

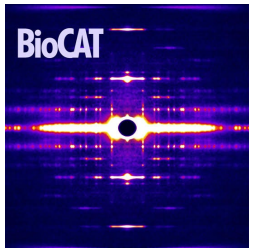
- Overhaul/replacement of many major beamline systems for another 20+ years of reliable operation:
  - Vacuum systems
  - Cryogenic system
  - Motor controllers
  - Backend experiment control software
  - Networking

- Improvement to vacuum systems in experimental hutch to reduce background, allow lower minimum q values



Planned upgrades

- New custom FPLC for SEC-SAXS to replace AKTA Pure
  - Fully integrated into beamline control software, allowing full automation of sample measurement, buffer changes
- Design goals:
  - Continuous unattended overnight running for SEC-SAXS samples
  - Full, automated temperature control from 4-50 C
  - In-line full spectrum UV measurement that also calibrates sample concentration in SAXS cell
  - Metal free sample flow path



Planned upgrades

- New batch mode autosampler
  - For samples where volume or concentration are insufficient for SEC-SAXS
- Design goals:
  - Direct loading into coflow cell to avoid dilution of sample
  - Loaded volumes as small as 10 uL
  - Fully automated loading for use with standard 96 well plates
  - Fully unattended running of batch mode samples