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**Proposal to Upgrade the BioCAT Beamline 18ID to a Dual-Inline Undulator A Configuration**

**The BioCAT Scientific Program**

The Biophysics Collaborative Access Team (BioCAT) is organized as A NIH-Supported Research Center dedicated to structural studies of partially Ordered biological materials using small-angle X-ray scattering (SAXS), small-angle fiber diffraction, and micro-X-ray absorption and emission spectroscopy (XAS). It is located at the Advanced Photon Source (APS), Argonne National Laboratory, Argonne, IL sector 18. The BioCAT facility is open to all researchers on the basis of peer reviewed research proposals. X-ray scattering and diffraction studies that have been addressed include static and time resolved macromolecular small-angle scattering, small and wide-angle diffraction of muscle, connective tissue, and oriented fibers of materials such as filamentous viruses. The BioCAT x-ray microprobe generates micron- scale beams ideal for interrogating the distribution of metals and their chemical speciation in tissue samples and other materials and their relation to human diseases such as neurodegenerative disease and cancer.

**Expected Impact of Proposed Upgrade**

All of our scientific programs could benefit from a two- to four-fold increase in flux. Perhaps our highest profile projects are with the Lombardi/M. Irving collaboration (University of Florence/ Kings College London). So far, this collaboration has resulted in one paper in *Nature* (Reconditi M, et al., 2004, *Nature* 428:578-81) and one in *Cell* (Piazzesi et al.,, 2007, *Cell* 131, 784–79) based on work at BioCAT. These projects use x-ray diffraction of single frog muscle cells. Achieving high time resolution requires adding up patterns from many 10's of contractions. Doubling the flux would allow these measurements to be done in half the time and, all other things being equal, double the rate of progress. Other time resolved experiments with M. Reedy Duke University, H Huxley, Brandeis, P. de Tombe, UIC would similarly benefit from the upgrade.

Another program that would directly benefit from increased flux would be time resolved macromolecular solution scattering using stopped flow. To obtain a satisfactory SAXS patterns requires 0.1 sec exposure with the photon counting Pilatus 100K detector. So to obtain 1 ms time resolution, with our current optics and flux levels requires 100 repeats. Every single repeat consumes a sample volume of 40 ul of a 0.4 -2 mg/ml concentration at a minimum. 100 repeats, therefore, will consume a sample volume of 4 ml and this represents a huge amount of protein and RNA that would be prohibitively expensive to produce for many systems. Again, a two-fold increase in flux would ½ the time to acquire such data and increase throughput by a similar amount but the most important benefit of increased flux is to reduce sample consumption. This could make the difference between go and no-go for experiments depending on the circumstances.

The program where increased flux would have the most dramatic impact would be our hard x-ray microprobe program. Here, throughput is limited by the need to obtain adequate counting statistics at a given point in a sample so that typical scan times are 1

sec/point resulting in an average of 3 hours per $mm^2$ of sample area). In rapid scanning mode, data acquisition overhead can be made not to be limiting, so that a factor of two increase in incident flux would result in a similar factor in throughput. This would mean that a given investigator could examine twice as many samples in the same time or two investigators could be accommodated in the time formerly used by one---both extremely desirable outcomes at our current oversubscription levels.

Increased throughput would be even more important with micro XAFS experiments. XANES acquisition times are typically one hour per pixel while EXAFS measurements require several hours per pixel (or per point) depending on the local concentration of the element of interest. These experiments are only performed on selected sample spots. Increasing the delivered flux by a factor of two would allow performing XANES measurements on more sample spots and it will make EXAFS measurements at micron scale on tissue samples more feasible. We are currently upgrading the KB optics to increase the flux by a factor of 3. An additional two-fold improvement would make a very significant improvement in throughput.

There are also competitive issues at stake. New SAXS beamlines are being built and commissioned at Soleil and Petra III with flux levels on par with the existing 18 ID. ID02 at the ESRF can already deliver approximately three times the flux of 18 ID when all three undulators in their straight section are in use. An upgraded source at 18ID would maintain its ability to compete with the state of the art.

**Proposed Upgrade:**

The most practical way to reach our goal would be to put an additional undulator A in the 18ID straight section in a tandem undulator configuration as discussed in TB45. As outlined below, this would involve minimal changes in the beamline and retain our current accessible energy range.

A possible alternative to this configuration that we have considered is to replace the current undulator A with an undulator with a 2.7 cm period as described in TB45, Appendix C. In this case, a single undulator would deliver a factor of two in brilliance and, presumably, delivered flux. It would also have an energy range, first harmonic, of ~5 -17 keV. Having access to higher energies by utilizing the first harmonic could be useful to us as radiation damage in muscle experiments appears to be lower at higher energies based on experiments done at SPring-8.

An issue with either configuration will be the increased power load on the optics. With either tandem undulator A's or the 2.7 cm device, the power loads on the optics will be similar at 7-8 keV as they are currently at 4 keV (the low energy cutoff of our optics). Since only a few percent of the experiments done on 18 ID use incident energies lower than this, one could implement the upgrade by simply modifying the control system to disallow lower energies. An advantage of the tandem undulator configuration is that the gap of the second undulator A could be opened up and lower energies could be accessed using the existing undulator A for spectroscopy experiments.

Assessing low energies with the 2.7 cm period undulator would (possibly) require upgrading the existing optics for higher heatloads. An upgrade path for beamlines of the Rosenbaum/SBC design for higher heat load optics has not been identified.
As BioCAT is currently organized, the beamline downstream of the shield wall is capital equipment owned by the Illinois Institute of Technology. At this point in time, the only mechanism available to BioCAT for paying for such upgrades would be through NIH. The next opportunity for seeking money from NIH for such an upgrade would be in 2011-2012.

**Estimated Costs**

These estimates would have to be provided by the APS since it involves only equipment upstream of the shield wall that they own.