A High-Energy Bending-Magnet Beamline

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Science

This proposal is to develop a bending magnet (BM) beamline for high-energy x-rays with additional white-beam capability. Four complementary experimental techniques will be featured: high-energy scattering with area detectors, high-energy scattering with a diffractometer and a point detector, energy-dispersive scattering, and high-energy tomography.

As a high-energy storage ring, the APS is very well suited to produce x-rays above 40 keV. A standard APS BM is a strong source of high-energy x-rays and it is possible to further "harden" the spectrum, perhaps in conjunction with a "long" straight section (see Borland, "Preliminary Study of a Strong Bend Option for the APS, APS OAG-TN-2004-003).

The use of high-energy x-rays to study the mechanical behavior of materials is discussed in a separate midterm proposal for the upgrade of the high-energy ID beamline capabilities. The beamline proposed here is complementary to that program. The ID program is moving towards using higher spatial resolution (< 10 microns) to measure different constituents in heterogeneous materials. The BM beamline would have larger beams and be used to probe macroscopic samples. Also, it is expected that time-resolved work would largely be carried out on the ID beamline and that the BM line would be for static samples. PDF experiments would follow a similar theme, with the BM beamline taking experiments that do not need the full power of the ID beamlines.

The amount of high-energy x-ray beam time available for experiments using a traditional diffractometer and point detector has dramatically decreased at the APS, largely due to tremendous growth in the demand for area detector experiments. However, there is a class of experiments that can only be done with a diffractometer and point detector. The magnetic and phase transformation experiments at 11-ID-C are examples of such research. The BM instrument proposed here would be a complementary tool to those experiments and could be used where flux requirements are somewhat relaxed. Another example is high-energy x-ray diffuse scattering, which sometimes requires a point detector to detect weak signals or to discriminate background scattering, but is often not flux limited.

Nearly all diffraction experiments at the APS are currently carried out using angular dispersion, either using area detectors or point detectors. It is also possible to measure diffraction using energy dispersion with an energy-resolving detector. This has the advantage that all scattering takes place into a small solid angle. This is a very attractive feature for studies in extreme environments where the need for large x-ray windows can compromise the environmental chamber. Also, energy-dispersive diffraction measurements can be made in such a way as to fix the gauge volume, which can be important in watching the evolution of heterogeneous materials (on example is the

cement research done at 1-ID a few years ago). As will be described below, detector advances open new opportunities for energy dispersive scattering experiments.

Exciting opportunities exist for using high-energy tomography at the APS. The instrument at 2-BM is limited to 30 keV, and there are many samples that require higher energies for sufficient transmission. Examples include heavier metals (e.g., Ni, Cu), fuel cells, many ceramics, and biological samples with highly mineralized tissue (e.g., bones and teeth). To look at highly absorbing samples with lower energies requires reducing the size of the sample, which is often not possible without compromising the experiment. High-speed tomography (such as that done at the ESRF ID15 beamline) and high-speed radiography (like that at 32-ID) are techniques with many scientific applications. A BM source cannot duplicate the high flux of an ID, but is still a potent source and will allow imaging of larger samples, though at a slower rate.

Added value to the medium term upgrade

The use of high-energy x-rays is well established at APS ID beamlines (1-ID, 11-ID-B&C, 6-ID) with strong oversubscription for user programs in this area (often more than a factor of 4). Most of the ID high-energy x-ray experiments need the high-brilliance from these beamlines. However, there is a significant subset of experiments that are of high science quality, but do not require such high brilliance. The spectrum from an undulator is strongly peaked at specific energies and is contained in a beam of small spatial extent. The former is fundamentally unsuited to energy-dispersive diffraction and the latter is problematic for imaging of larger samples.

Over the past few years, the use of large area detectors has come to dominate high-energy x-ray experiments at the APS ID beamlines. Other midterm proposals concerned with upgrades for ID beamlines at the APS detail the need for fast, large area detectors (e.g., the GE detector), and the science that will be enabled through their more ready availability. As such detectors become available, the ID beamlines will move increasingly toward experiments emphasizing sub-second time resolved data collection. This leaves an experimental niche for a high-energy BM beamline. Currently, a lot of very nice science is being done in both the PDF and strain/texture areas using the Mar 345 image plate (~1 minute readout times), and there is no indication that the demand for this capability will diminish anytime soon. A high-energy BM instrument can address most of this need, working both to produce science directly and to serve as a step towards the more advanced time-resolved experiments on the ID beamlines.

With the growth of the use of area detectors for high-energy x-rays, the use of diffractometers and point detectors has consequently decreased. These experiments tend to take considerably longer per data set and often require considerably more expertise by the user to execute. However, there are many scientific studies best addressed in this way. For experiments with weak experimental signals, point detection with energy discrimination (either through an analyzer crystal or high energy resolution detector) is sometimes essential. Often these experiments are not brilliance limited and the flux from a BM would be sufficient, albeit with longer data acquisition times.

A dedicated energy-dispersive scattering setup would add a useful tool to the suite of APS instruments. The smooth energy spectrum of a BM is very well suited to this technique. With currently available detectors (i.e., solid-state Ge or Si detectors), the main advantage of this technique is the ability to measure a diffraction spectrum from a small solid angle. This is particularly useful for examining samples in extreme environments (e.g., very high temperatures, high pressures) allowing for a much smaller x-ray window. The energy resolution limits the accuracy of d-spacing determination, but often very valuable information on phase evolution can be obtained.

It appears that superconducting tunnel junction (STJ) detectors (also called transition edge sensors—TES) are on the verge of causing a quantum leap in the utility of energy dispersive methods. The demonstrated energy resolutions from these detectors allows d-space determination that is equal to or in some cases better than that with large area detectors. The issue with these detectors is that their maximum count rates have always been much better suited to astrophysics applications than the high count rates of synchrotron scattering experiments. Pixelation of STJ detectors has allowed the count rates to be dramatically increased. This has yet to be demonstrated at high energies, but is in principal straightforward. In the time frame of realization of this proposal, such detectors may become available and, if so, radically change how we take data for a variety of experiments. Depending on undeveloped technology is inherently risky, and hence the approach of this proposal—to provide an instrument that can use this technology if it becomes available, but to provide a useful, working instrument if it does not.

Finally, the XOR tomography setup at 2-BM is limited to 30 keV by the 2-BM optics. This beamline has a large and growing user program that is well served by this energy range. However, a higher energy tomography instrument would allow experiments on a new range of samples that are too absorbing for the current setup. The white beam tomography and radiography will complement the imaging program at 32-ID. The imaging instrument proposed here will be fully integrated with the existing computational infrastructure already existing in XOR for high throughput tomography and therefore highly synergistic with other existing XOR programs.

Expected user communities

The proposed beamline will be used by the large, established high-energy community at the APS. It will be of benefit to both the mechanical behavior users of 1-ID and the broad PDF community of 1-ID, 6-ID, and 11-ID B & C. We would expect the current users of the 2-BM tomography program to use the high-energy tomography, and that users of the 32-ID white-beam imaging program would also be able to use the new beamline.

Enabling technology and infrastructure

We propose building a BM beamline for high-energy x-ray scattering and high-energy tomography with white beam. No such beamline currently exists at the APS. Given that there are several available APS BM ports, it would probably be best to build this

beamline on a greenfield site, but it would also be possible to retrofit a currently built beamline (e.g., 1-BM). If BMs are modified at the APS to have stronger magnets (e.g., for a longer straight section ID beamline), such a sight would obviously be beneficial for the proposed beamline.

The beamline would have three stations: a first optics enclosure, a white-beam station, and a monochromatic station. The first optics enclosure would have two major optical components—a multilayer mirror (for high-energy tomography) and a double-crystal, sagittal focusing monochromator. The white beam station will need to be fairly large, with enough room for a tomography setup and an energy dispersive scattering setup. Both would be sensitive instruments with considerable setup and would be permanently installed at the beamline. Monochromatic station will be placed as far downstream as possible to help with the focusing of the high-energy x-rays. The monochromatic station will have two setups: one for scattering with a large area detector and a second for a diffractometer using a point detector.

The optics for this beamline present some challenges and will require some R&D, but current APS staff are well suited for this effort. The experimental instruments will be largely copied from existing, successful APS programs. The exception is the energy-dispersive scattering setup. A prototype for such an instrument was used at 1-ID several years ago, with promising results. The effort was curtailed due to the disruption caused to the overall 1-ID beamline operations. A permanent location for the instrument will alleviate that problem.

As with the ID beamlines, key to the area detector experiments is a large, low noise, 2-D detector that is reasonably efficient at high-energies. Readout speed is key for the ID experiments, where the mismatch between data collection times and readout times if very poor. Speed is also desirable for a BM instrument, but here it is less crucial. We would expect that the area detectors used on the BM would be ones that are no longer in heavy demand by the ID programs; in essence, one generation behind the state of the art.

As described in other high-energy midterm proposals, ancillary equipment is very important for high-energy x-ray scattering. The beamline requested in this proposal is heavily leveraged in this respect because all of the needed equipment is already being developed for the ID beamlines and can be borrowed or copied. The same situation exists for data handling and analysis. In particular for high-energy tomography, where the infrastructure for reconstruction of the images is already developed for the 2-BM program.

Partnerships and user interest

For the proposed beamlines, we will partner with the XOR ID high-energy programs, the 2-BM tomography program, and the 32-ID white-beam imaging program. The users of those beamlines will also be interested in this beamline.

<u>Industry</u> and technology transfer

The proposed beamline has considerable potential for industrial research. Development of such a community would depend on strategic decisions of APS management towards this purpose.

Estimated Budget

We estimate approximately \$3M for a new bending magnet beamline. For instruments, \$300K for the diffractometer system, \$200K for the area detector instrument (not including the detector, which could be an existing in house detector), \$200K for the energy dispersive setup, and \$250K for the imaging equipment. (Total = \$3.95M.) Front end and storage ring costs not included.