Beamline Upgrade Proposal
Medium-Term (5 year) Plan for APS Beamline Improvements and Enhancements

Canted Undulator Upgrade for GeoSoilEnviroCARS Sector 13

March 28, 2008

Summary

GeoSoilEnviroCARS (Sector 13) is a heavily oversubscribed, national user facility for earth, planetary and environmental science research supported by NSF-Earth Sciences and DOE-Geosciences and is open to the entire scientific community through the APS General User program. A canted undulator upgrade is proposed which will support a unique sub-micron microprobe, provide an optimized x-ray source for mineral-water interface and high pressure diffraction studies, and double the undulator beam time available to users.

Science

The impact of the upgrade to the APS science program will be threefold. First, a unique sub-micron microprobe with optimized undulator source will be available in a dedicated station for nearly simultaneous, chemical speciation analyses on light (as low as sulfur) and heavy elements in systems of geochemical, environmental and cosmochemical significance. Second, a companion undulator optimized for high energy will added to advance the quality of mineral-water interface and high pressure diffraction data. Third, the doubling of undulator beam time will open up the capabilities of GeoSoilEnviroCARS to many more investigators than currently possible.

The ability to access S, Cl, K, and Ca K-edges as well as K and L edges of heavy metals with a single sub-micron microprobe will be a unique capability at the APS and will offer tremendous new opportunities for science in geochemistry, cosmochemistry and environmental science. Access to the sulfur K-edge is particularly important for many environmental and geological systems, such as those associated with mine waste tailings, metal contaminated aquifers (e.g., those in Bangladesh), and meteorites from Mars.

The availability of the optimized high energy undulator radiation will greatly improve the quality of experimental data on how the structures of mineral surfaces influence the mode(s) of sorbate binding under environmentally relevant conditions. Such information is critical in developing a fundamental understanding of the chemical reactions that control the fate of contaminants in natural aquatic systems. High brilliance and flux at high energy will also enhance the quality of high pressure experiments, useful in exploring the nature of the Earth's interior as well as the structures and properties of novel materials.

The increase in available undulator beam time will advance all our frontier science including high pressure mineral physics and chemistry, properties of melts and other non-crystalline and nano-crystalline materials at high pressure, chemistry and physics of hydrothermal fluids and magmas, inorganic reactions at mineral-water interfaces and other environmentally-relevant processes, biogeochemistry, flow dynamics of fluids and solids, and cosmochemistry.

This research addresses priorities documented in the DOE-BES report "Basic Research Needs for Geosciences: Facilitating 21st Century Energy Systems" (2007), specifically, the priority research directions of "Mineral-Water Interface Complexity and Dynamics", "Nanoparticulate and Colloid Chemistry and Physics", and "Biogeochemistry in Extreme Subsurface Environments."

Added Value of the Upgrade

The existing single Undulator A will be replaced by two optimized undulators: the first optimized for 2.3-23 keV (possibly polarization adjustable) and the second for 5-100 keV. Total available undulator beam time will be doubled allowing a dramatic increase in the size of the user community. Microprobe capabilities will be enhanced in several ways. First, the energy range will be extended to lower energy.

Second, the focal spot size will be reduced and made easily tunable via implementation of a secondary focus geometry.

Expected User Communities

GeoSoilEnviroCARS has become continuously oversubscribed predominately by earth, planetary and environmental science users. Over 700 unique users have conducted experiments. The oversubscription factor, defined to be the ratio of the number of days requested by users to the number of days awarded (= number available), has averaged about three (i.e., 300% subscription) for 13-ID over the last five years. In the most recent cycle (2008-2), the oversubscription factor on 13-ID was 3.3. With the canted undulator upgrade, we expect an expansion of the user community in all areas but particularly the addition of new users interested in the speciation of light elements and coupled studies of light and heavy element speciation. Over the last five years GeoSoilEnviroCARS has more publications than any other non-macromolecular crystallography sector at the APS, according to the APS Publication Database. This proposed upgrade will allow us to further improve on the productivity of this facility.

Enabling Technology and Infrastructure

The conceptual design involves installation of two new undulators, one optimized for supplying 2.3-23 keV x-rays to a dedicated sub-micron microprobe station (produced by subdividing the existing 13-ID-C station) and the other optimized for 5-100 keV operations for high pressure and interface diffraction science. The beam from the intermediate energy device will be deflected by dual deflecting mirrors providing an undulator beam separation of 13 mrad (Figure 1). The sub-micron microprobe beamline will be operated in a horizontal compound focusing geometry to allow continuously adjustable beam sizes from 250 nm to 4 μm containing 2 to 30% of the undulator fundamental, respectively. The

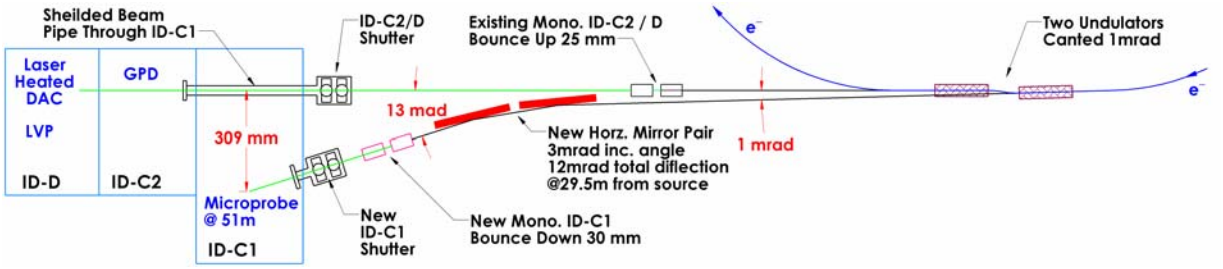

Figure 1: Schematic for the proposed Sector 13 canted undulator mode upgrade.

availability of two undulators in a canted geometry will allow simultaneous and independent operation of two undulator experiments, doubling the undulator time available to the users.

With help from the APS Magnetic Device group (E. Moog, R. Dejus) and assuming a 11 mm gap and currently achievable magnetic field strengths, calculations of on-axis brilliance were done for APS Undulator A (33 mm, 72 periods), a 33 mm device with 62 periods (Undulator A, modified for canted mode), a 36mm device with 57 periods, and a 29 mm device with 70 periods. Figure 2 shows the on-axis brilliance for harmonics 1 to 7 of these devices. The 36 mm device can reach 2.240 keV, well below the S K-edge and maintain brilliance above 10^{19} past 25 keV. The 29 mm device can reach 5.600 keV, well below the Cr K-edge, and has higher brilliance than Undulator A between 5.6 and 13 keV and above 20 keV. As with any short period device, there is a tuning gap for this device between ~15.5 and 16.8 keV. Importantly, this still allows access to the uranium LIII-edge at 17.166 keV.

We will also explore the feasibility of designing the intermediate-energy undulator to be polarization adjustable. It is well known that the linear polarization of the synchrotron x-ray beam can complicate the interpretation of XAFS on non-cubic mineral phases for oriented single-crystals, and that XANES is affected by the mineral orientation. While measuring multiple orientations of a well-oriented

sample or spinning the sample can mitigate these effects, this approach is not feasible for microprobe work. An alternative is to illuminate the sample with circularly polarized light. This will allow us to collect plane-polarization-averaged XANES on randomly oriented micro-crystals and greatly reduce the potential artifacts of unfavorable orientation of the crystal axes with the x-ray beam.

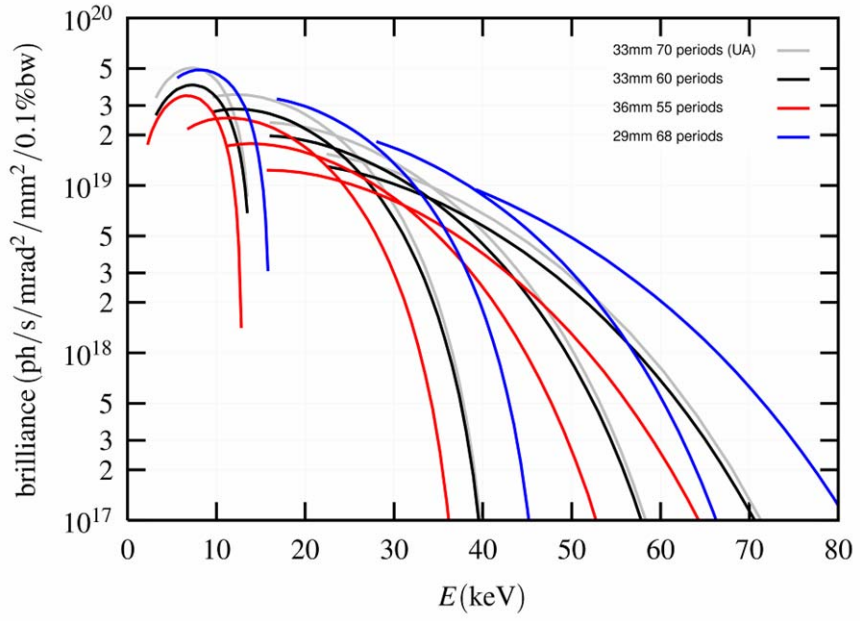

Figure 2: The on-axis brilliance plotted for the 1st to 7th harmonic of Undulator A (grey line), a 33mm period undulator for a canted beamline (black line), a 36 mm period undulator for the intermediate energy beamline (red line) and a 29 mm period undulator for the high energy beamline (blue line).

Summary of Upgrade Modifications

- Undulator 1 (design, fabricate, install): 2 m, 2-23 keV, possibly adjustable polarization
- Undulator 2: (design, fabricate, install): 2 m, 5.5-100 keV
- Front end (design, fabricate, install): canted ID components
- Flat deflecting mirror (design, fabricate, install): silicon, 700 mm, power handling component.
- Bendable deflecting mirror (design, fabricate, install): silicon, 500 mm
- Monochromator for 13-ID-C1 line (design, fabricate, install): Si(111) double crystal, water cooled, bounce down.
- Monochromator for 13-ID-C2 line: modify to pass 13-ID-C1 beam
- Shutters for 13-ID-C1 and 13-ID-C2 (design, fabricate, install):
- Station 13-ID-C modifications: install interior wall, install new door for 13-ID-C1
- Beamline KB mirrors (13-ID-C2): move to new locations in 13-ID-B and 13-ID-C2
- Shielded pipe in 13-ID-C1 (design, fabricate, install)
- PSS and EPS upgrades

Project Management

The sector upgrade will be managed by the GeoSoilEnviroCARS staff (all University of Chicago employees) in collaboration with the APS staff. GeoSoilEnviroCARS is a national consortium managed by two Project Managers (M. Rivers and S. Sutton) and six Technical Groups organized around the six

principal techniques in the sector. Each of these groups has a GSECARS staff member as a leader as shown below:

- Diamond Anvil Cell (Vitali Prakapenka, Senior Research Associate)
- Large-Volume Press (Yanbin Wang, Senior Research Associate)
- Microtomography (Mark Rivers, Senior Scientist)
- X-ray Absorption Fine Structure Spectroscopy (Matt Newville, Senior Research Associate)
- X-ray Diffraction and Scattering (Peter Eng, Senior Research Associate)
- X-ray Fluorescence Microprobe (Stephen Sutton, Senior Scientist)

These individuals have the responsibility to lead the development of science, instrumentation and user community in their particular area, oversee the maintenance of instrumentation and work to satisfy software needs. In addition, the leaders work closely with users to ensure the success of experiments (experiment design, experiment conduct, data analysis, etc.) and receive input from them on potential new technical directions.

For the upgrade project, Peter Eng will be the Project Leader with the assistance of the rest of the GeoSoilEnviroCARS staff. Peter has developed the conceptual design presented in this document and is the principal staff member responsible for optics and beamline development at GeoSoilEnviroCARS. Sector 13 has been completely designed, installed, commissioned and operated by GeoSoilEnviroCARS staff.

Industry and Technology Transfer

We anticipate newly developed optics, such as the deflecting mirrors, to be made available to the at-large synchrotron radiation community. Such technology transfer of GeoSoilEnviroCARS products has occurred previously. In order to focus the APS source to a few microns, Peter Eng developed a pair of very asymmetric, elliptical Kirkpatrick-Baez mirrors capable of focusing either white or monochromatic x-rays. A scalable bender mechanism was developed, and made available to other institutions through the University of Chicago machine shop. The success of this microfocusing device is demonstrated by the more than 20 copies of the bender design that have been deployed around the ring of the APS, at the NSLS, at the Beijing Synchrotron, and at CAMD. The large, water-cooled Kirkpatrick-Baez mirrors in 13-ID-B were also designed and constructed by Peter Eng. This design is being sold commercially by IDT and these assemblies are now installed at HP-CAT at the APS, at the Swiss Light Source, the Canadian Light Source, and will be installed at Diamond.

Estimated Budget and Timeline

The proposed expansion involves the development, installation and commissioning of components within the synchrotron storage ring (new undulators, dual beam front end, etc.) as well as instruments as part of the beamlines (monochromator, mirrors, shutters, experimental hutch modifications). The “behind-the-shield-wall” upgrades will be equivalent to ~$1.5M. The “beamline” upgrades are estimated to be ~$2.0M for a total cost of ~$3.5M. These funds are likely to be required over a two year period.

These upgrades can be achieved with minimal impact and interruption to the existing scientific program. An aggressive phase-in plan has been developed making use of three consecutive machine maintenance periods (four to five weeks in length) allowing all of the required optics and infrastructure to be installed with the user program resuming without interruption after each of the first two periods. After the third and final installation period approximately one to two weeks of beam time will be required to commission the new optics and stations.

Letter of Intent to the APS SAC

GSECARS submitted a canted undulator upgrade Letter of Intent to the APS Scientific Advisory Committee for their consideration at their January 2007 meeting. In June 2007, we received a very positive response from the APS Director, J. Murray Gibson. Dr. Gibson’s letter is attached as well as the Letter of Intent, which contains additional details of our proposed upgrade.