# Report of the HPCAT Advisory Committee:

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| Date of meeting: | June 1, 2015 |
| Location of meeting: | Advanced Photon Source, Bldg. 434, Rm. C010 |
| Committee members: | Wolfgang Sturhahn (Chair), California Institute of Technology<br>Michael Desjarlais, Sandia National Laboratory<br>Tom Duffy, Princeton<br>Chi-Chang Kao (not present), SLAC National Accelerator Center<br>Martin Kunz, Lawrence Berkeley National Laboratory<br>Mark Rivers, University of Chicago<br>De-Ming Shu, Argonne National Laboratory<br>Choong-shik Yoo, Washington State University |

The Advisory Committee (AC) met on Monday, June 1 with HPCAT executive director (V. Struzhkin), management, (G. Shen, S. Sinogeikin), the HPCAT Executive Committee members, as well as HPCAT staff. The morning was devoted to presentations on current status as well as on a three-phase upgrade plan taking into account the possible upgrade of the Advanced Photon Source (APS) storage ring to a diffraction limited multi-bend achromat (MBA) "ultimate" storage ring. The Advisory Committee then discussed the following charges in the presence of Guoyin Shen and members of the HPCAT Executive Committee.

1. HPCAT facility – capabilities and competitiveness in the world;
2. HPCAT operation – productivity and quality;
3. HPCAT overall direction – future outlook;
4. HPCAT near future development projects (next 5 years) – advancement and reasonableness;
5. HPCAT upgrade plan with MBA lattice – preparedness and potential impacts.

A brief summary of the AC's assessment regarding these topics was presented at the end of the meeting and is repeated at the beginning of each topical section.

The Advisory Committee was generally impressed by the performance of HPCAT which operates four beam lines simultaneously at highest level. This is remarkable given the complexity and variety of different experimental techniques offered, and the excellent overall quality reflects positively in the publication record. The work-planning process for user experiments is very well organized, e.g., a local contact assigned to every user experiment and additional support is available during the actual beam time. This results in an efficient distribution of the workload among the scientific staff and gives individual staff members the opportunity to collaborate with various user groups. The committee is especially impressed by the staff performance in view of lower staffing levels than found at beam lines with comparable focus and performance, e.g., at international high-energy storage rings such as the ESRF and SPRing-8.

The three-phase upgrade developed by HPCAT provides a very sensible path to technical improvements that are required to address long-standing as well as novel problems in high-pressure science, e.g., precise equations of state and melting temperatures, electronic properties of H/Li/Na, strain-rate dependences, poly-amorphism is glasses and liquids, static pressures in excess of 5 Mbar.

## 1 Capabilities of facility and competitiveness in the world

Summary: The technical capabilities are world class and truly impressive. Several developments are world leading and can be expected to be followed by others. Achieving a facility of this quality would not have been possible without 15 years of consistent funding.

HPCAT operates four beam lines simultaneously at highest level. A second undulator in a canted arrangement was recently added to support two completely independent ultra-high brilliance beam lines. One branch is dedicated to flux-hungry spectroscopies such as x-ray emission (XES), inelastic (IXS), and nuclear resonant (NRS). The other branch is highly optimized for micro-diffraction studies with environmental support such as Laser heating and cryogenic cooling. The bending magnet emission fan is spatially split and delivers x-rays for two stations. One of them is dedicated to x-ray absorption spectroscopies and micro-diffraction, the other station offers white-beam Laue and energy-dispersive x-ray diffraction. All beam lines feature micro-focusing to accommodate studies on very small samples.

With these excellent experimental capabilities crystal structures and electronic states of matter are characterized under extreme conditions of pressure and temperature. The quality of the resulting data are superb and largely justify a world-class status of HPCAT as an experimental high-pressure facility. The study of phase-transition kinetics under rapid compression and de-compression as well as under conditions of modulated Laser heating is a novel and potentially ground-breaking addition to HPCAT's capabilities. This particular aspect can certainly be considered world-leading. At present the development of time-resolved studies reaches time-scales down to milli-seconds, but it appears that micro-second time scales are attainable with appropriate upgrades.

The development and successful operation of such a multitude of experimental capabilities was possible through stable and dedicated financial support over the last 15 years. The Advisory Committee hopes that changes in the funding structure for HPCAT with DOE-NNSA now providing 75 % of funds for HPCAT operations would have no discernible negative impact on the HPCAT facilities capabilities and staffing.

## 2 Operation – productivity and quality

Summary: HPCAT has highly qualified and motivated staff, an excellent publication record, and a high level of technical development. The high number of innovative projects could influence the balance between R&D and user support. This balance should be carefully monitored to maintain a high level of user satisfaction.

HPCAT has built and maintains are highly effective support structure for user experiments. Highly qualified and motivated staff and an extensive selection of support equipment and laboratories are key ingredients for the high quality of HPCAT's scientific productivity. The user experience at HPCAT is notably enhanced by a local contact person, high reliability of beam line optics and support equipment, and robust instrumentation in accessible areas. The local contact is responsible for smooth interaction with scheduled users including communication and discussion of experimental procedures prior and after an experiment. During the experiment the entire HPCAT staff is available to support the successful execution of the experimental plan. This results in an efficient distribution of the workload among the scientific staff and gives individual staff members the opportunity to collaborate with various user groups. Backup equipment for critical beam line components and computing resources significantly shortens potential downtimes caused by equipment failure.

The personal safety of users and staff as well as operational safety are well managed through interlock systems, engineered feedback systems, and clearly spelled out specifications for particular experimental setups.

Beam time allocation is distributed between HPCAT partners (60 %), the general APS user population (25 %), and internally for beam line readiness and R&D (15 %). The number of users has been relatively constant over the last six years indicating a certain level of maturity. Nevertheless the number of refereed publications has steadily increased over the same time period to about double the number in 2009 indicating a steady increase of productivity. The publication record is supplememented with other outreach activities such as the organization of scientific meetings, summer schools, and the APS-local high-pressure interest group.

In light of these developments, the committee is especially impressed by the staff performance given the somewhat lower staffing levels than found at beam lines with comparable focus and performance, e.g., at international high-energy storage rings such as the ESRF and SPRing-8. HPCAT recently engaged in several innovative projects with potentially great impact on high-pressure science. In light of this additional activity, an impact on productivity and user satisfaction (which is very high) may be unavoidable at similar staffing levels.

## 3 Overall direction – future outlook

Summary: The synergistic approach of HPCAT has been successful to provide excellent scientific results. Additional techniques such as single-crystal or multi-grain diffraction probably require additional effort in software development and user training to attract a broad user base and potentially replace powder diffraction.

HPCAT provides a large variety of x-ray scattering techniques to its users. This multi-pronged approach to address scientific problems has been very successful over the years. A recent special collection of papers published in RSI describes the status-quo at HPCAT as well as new developments. In this context, HPCAT has added new capabilities such as single-crystal or multi-grain diffraction to its expanding portfolio of experimental techniques. These developments are very exciting because they could replace the very popular powder diffraction technique for exceedingly small x-ray focal spot sizes, e.g., incase of the MBA upgrade.

For HPCAT, it seems natural to strive for an even larger portfolio of experimental techniques to continue this line of success. As HPCAT also realizes this expansion process, even though desirable for many users, is resource limited. For example, the replacement of powder diffraction with equivalent or superior techniques requires not only instrumental development, but also the creation and testing of evaluation software and very importantly the training of users in efficient use of the new techniques.

## 4 Near future development projects (next 5 years) – advancement and reasonableness

Summary: We agree with the three-phased upgrade of HPCAT, and all presented plans are very reasonable.

The emphasis on x-ray detectors in Phase-I of HPCAT's upgrade plan is a great way to optimize data collection but also to explore new applications such as time-resolved micro-diffraction. Improved focusing optics can provide spot sizes sufficiently small for scanning of samples in diamond-anvil-cells. In either case, new scientific opportunities will emerge, and HPCAT has developed a vision that creates connections between instrumental developments and scientific problems.

Technical progress (fast efficient detectors, more precisely machined mirrors and capillaries, new compression devices) leads to enhanced instruments that are then integrated into a new capability to benefit the user base and high-pressure science. HPCAT advances this dynamic process of interwoven areas very well with an eye on the needs and requests of their users and funding agencies.

## 5 Upgrade plan with MBA lattice – preparedness and potential impacts

Summary: Even though HPCAT is quite well prepared to address the improvements and changes expected from an APS upgrade to a low-emittance MBA lattice, we would need to hear more evidence about resulting transformational science, for example, from coherent diffraction or imaging approaches.

The present upgrade plan of the APS is driven by a change of the magnetic lattice of the storage ring to a multibend achromat (MBA) design. The implementation of the MBA is expected to reduce the horizontal electron emittance significantly. This should then lead to x-rays with much smaller divergence emitted by a smaller source, i.e., a vastly increased brightness leading to a significantly more coherent beam. With present undulators, the x-ray flux would be similar or even reduced because of the lower electron energy in the storage ring (6 GeV instead of todays 7 GeV). This situation can potentially be improved by installing superconducting undulators with shorter magnetic period than todays devices. The on-sample flux however could increase substantially if focusing devices captured a larger fraction of the x-ray beam than at present. In summary, the major change resulting from the MBA upgrade would be a smaller, more coherent x-ray beam.

HPCAT projects that the MBA upgrade is realized in about six years from today and has developed a specific upgrade plan with activities starting about three years before the MBA upgrade. This is a reasonable starting point in time which however may recede determined by the APS upgrade schedule. The MBA related upgrade appears to be Phase-II of HPCAT's overall development strategy. Phase-II emphasizes the improvement of beam delivery optics to adjust to the x-ray beam quality and, in particular new focusing elements to take advantage of the higher brilliance of the x-rays. These are very sensible steps in the MBA scenario.

Under the MBA upgrade plan of APS, bending magnets are replaced with 3-pole wigglers that deliver significantly more x-ray flux at energies above 20 keV. In HPCAT's Phase-II plan, this situation is exploited with a re-design of the bending magnet beam lines emphasizing high-energy micro-diffraction of solids and liquids which would be a very fruitful development.

In Phase-III of HPCAT's upgrade plan, the introduction of new x-ray techniques is envisioned. Such techniques presumably require a degree of coherence that is not available today but would be provided by an APS storage ring with the MBA-lattice. The addition of coherent diffraction and/or x-ray imaging to HPCAT's portfolio sounds intriguing. Here the Advisory Committee encourages HPCAT to further study the nature of these techniques in the framework of high-pressure science. Any evidence that transformational science could result would clearly strengthen the case of this aspect of HPCAT's upgrade plan.