Report of HP CAT Review March 5, 2013

Submitted June 21, 2013

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Brief Synopsis

HPCAT operates two beamlines (16-ID and 16-BM) at the APS dedicated to high pressure research encomposing materials, solid state and geophysical sciences. The main membership consists of the Carnegie Institution of Washington, Lawrence Livermore National Laboratory, Los Alamos National Laboratory, Sandia National Laboratory, University of Nevada at Las Vegas, and CDAC (a consortium of universities with interests in high pressure research). Funding has been stable at approx. 3M$/yr of which 75% comes from DOE-NNSA via Carnegie, and 25% from DOE-BES. General user proposal (GUP) time is 25%.

Scientific operation is very impressive with roughly 80 publications per year including many in high impact journals, a similarly impressive distribution of users from around the world, and several very important scientific findings over the review period. The facility has a remarkably broad range of techniques represented, many available in synchrony at a single beamline. The facility is competitive with analogous sets of beamlines at other world facilities, but has a unique integration of capabilities. Additionally, HP-CAT has an outstanding technique development record, which is closely connected with a noteworthy ability to train new scientists in high pressure synchrotron science.

Staffing appears adequate to continue to achieve at these levels, but there is evidence of strain, especially in consideration of new initiatives, and there is an issue with individual career development, for which no independent beam time for research is currently allotted. Management is through an executive committee that makes all critical decisions. A scientific advisory committee, which meets and is appointed at the discretion of the executive committee, seems to have a minor role, having met only twice over the last four years. Future plans, including the development of submicron beam capabilities, are very well coupled with the goals of the APS upgrade. Although challenging, they appear to effectively utilize existing expertise at other APS beamlines to good advantage. Other challenges include a better coupling to theoretical analysis involving several types of studies, and software development, which appears to trail new technique implementation in priority.

Detailed Analysis

Scientific Performance and Productivity

HP-CAT has produced impressive scientific research achievements over the review period, evidenced by a strong publication record, an outstanding production record for student theses, and many notable scientific findings. Some of the most significant science described during the review and/or contained in review materials supplied by the APS include: New descriptions of the ordered state in amorphous metals and carbon clusters (Science, 2012; Science, 2011); f-electron delocalization and volume collapse in metals (PRL, 2012; PRB, 2012); the reappearance at high pressures of superconductivity in iron arsenides (Nature, 2012); new complexity in the phase diagram and structural transitions in alkali metals (Nature Physics, 2011).

The publication record is among the best for any sector at the APS, averaging about 76 publications (journal articles, book chapters, student theses) a year, with the journal average alone (about 60 per year) comparing favorably with other strong sectors such as GSECARS. The number of theses (MS and PhD) average about 10 a year, which is exceptional. The fraction of publications in high impact journals is also noteworthy, with roughly 17% of journal articles in generally accepted high impact publications (based on APS-supplied information). Involvement in international conferences and workshops is significant, and appears to be in accord with the other high level scientific metrics.

Management Structure and Performance

Management of HPCAT is via an executive committee (EC) comprised of representatives of the main constituency. At present committee members include H.K. Mao (Executive director), R.J. Hemley (CIW), S. A. Gramsch (CDAC), Y. Zhao (UNLV), W. J. Evans (LLNL), N. Velisavljevic (LANL), W. Yang (HPSync) and the HPCAT director G. Shen. G. Shen replaced H.K.Mao as HPCAT director in 2009, while H.K. Mao directs the EC. The EC meets at least 4 times annually with the HPCAT director to arrive at operational and strategic decisions.

A HPCAT advisory committee, appointed by and holding meetings at the discretion of the EC, advises on scientific plans, development feasibility, and enhancements of existing capabilities. This committee has met only twice in the past four years, and does not appear to function with a purview or charge akin to the SAC for the APS, or as advisory groups do for other CATS. Current advisory members are C.C. Kao (SLAC), M. Rivers (CARS), W. Sturhahn (Caltech), M. Kunz (LBNL) and D. Shu (ANL). The role of this committee was discussed with several of the current members.

Funding for HPCAT has been consistent over the review period with a small increase. 75% of funds are derived from DOE-NNSA and 25% from DOE-BES, although post October 2012, the 75% from NNSA comes directly via an agreement with CIW, whereas prior to this date the NNSA funding came via the three NNSA-supported partners (CDAC, UNLV, LLNL). The DOE-BES funding is via a separate grant to CIW.

Performance of management is judged by reference to several criteria treated separately: use of APS-supplied beamtime; general user satisfaction; capabilities and sector development; future planning; adequacy of funding; staffing

APS beamtime usage

The four stations at HPCAT are fully utilized, with up to 43% oversubscription on 16-ID-B according to APS User Office supplied information. This is actually a low oversubscription rate for the APS as a whole. However information supplied by HPCAT conflicts with the User Office information and suggests more expectable to very high oversubscription rates, probably as a result of differences in the calculation using the same base numbers, or from a different metric (e.g. use of requested time on a different basis). For example, 16-ID-B has approximately a 700% oversubscription rate from 2010-2013, while the other stations have from 150% to 360% oversubscription rates. It is recommended that the actual general user subscription rates be recalculated by the User Office and normalized to the same metric used with other CATs. Discussions with staff indicate that the beamline stations are heavily used, and tight schedules must be maintained to afford reasonable fractions of time for development and commissioning of facilities.

General user satisfaction

The technical and scientific staff appears highly knowledgeable and very responsive to diverse users' requirements, and particularly to general APS users. Users seem quite satisfied with the data obtained from the HPCAT end stations, both in terms of quantity and quality. The APS USER Office supplied feedback from approx. 144 users who had submitted end-of-experiment (EOE) reports on their experiences, about 70 of whom made specific comments, all very complementary to the staff, and to the quality of the facilities. The proportion of users indicating successful or highly successful runs at HPCAT was about 80%, with the remaining fraction almost universally indicating partially successful runs. The apparent time between data acquisition and publication was very reasonable, also consistent with an organized and well-supported user program.

Current Capabilities and sector development

HPCAT has pioneered the concept of "integrated synchrotron radiation experiments" dedicated to compression science and technology to study matter at extreme conditions. X-ray probes were conceived, developed, and implemented to enable the studies of physical properties of dense matter. Structural, vibrational, electronic, and magnetic properties can be probed at high pressure and high/low temperature using the instrumentation housed in the HPCAT end-stations.

The experimental capabilities are spread over four different beam stations at Sector 16. Each station is equipped with different end-station capabilities. Two stations take advantage of a canted undulator source providing very high brilliance in the 5-40 keV range. The high brilliance ID beamline serves four different end-stations for x-ray spectroscopy, i.e., x-ray emission spectroscopy (XES), inelastic x-ray scattering (IXS), nuclear resonant inelastic x-ray spectroscopy (NRIXS) at stations ID-C/D/E, and micro-

diffraction at high pressure and high/low temperature at station ID-B. Two other stations make use of a split x-ray beam arising from the bending magnet source (BM). At the BM three end-stations allow for diverse scattering and spectroscopy experiments: micro-diffraction (both powder and single crystals) and x-ray absorption near edge structure (XANES) spectroscopy at stations BM-C/D and white beam Laue diffraction and large volume x-ray scattering at station BM-B. Whereas the BM stations accommodate experiments carried out at modest and high pressures, using diamond anvil and large volume Paris-Edinburgh pressure cells, and variable temperature using cryocooling or resistive heating of samples at high pressure, the ID stations are mostly used for experiments at extreme pressure and temperature conditions, with samples in diamond anvil cells probed by x-ray beams at small scale (less than 10 mm) and at pressures exceeding 100 GPa with simultaneous temperatures ranging from 5 to 5000K using cryostats or laser heating. HPCAT has played a leading role in developing techniques to probe samples at extreme conditions with synchrotron radiation beams.

It is obvious that considerable effort is devoted by staff to optimize synchrotron beam usage, and enhance the general user's experience. Hardware, data acquisition software and graphical user interfaces, and data analysis software allow rapid and efficient gathering of high-quality data. As added user's support, HPCAT also provides ancillary equipment located both at the beamlines and in adjacent laboratories, e.g., spectroscopy systems for pressure measurement and Raman scattering, cryostats, and pressure cell preparation and control, and sample loading equipment. The suite of experimental capabilities available at the HPCAT also is enhanced by other complementary capabilities offered at several other APS beamlines which interact with the HPCAT staff (e.g. GSECARS).

It is thus our finding that the HPCAT Facility at the Advanced Photon Source represents a world-class platform for condensed matter science at extreme conditions. The Facility offers a remarkable suite of scattering and spectroscopy experiments utilizing hard X-rays from both bending magnet and insertion device sources. At present, nowhere else in the world does such a plethora of x-ray scattering and spectroscopy instrumentation devoted to high pressure science exist "under one roof". In this respect, and for the quality of its installations, HPCAT is to be considered the leading synchrotron radiation facility dedicated to science at extreme conditions.

Future Directions

The principal research directions presented by the HP-CAT Director, Prof G. Shen, are:

- Reaching 0.5 TPa and beyond – structure, bonding and thermodynamic properties
- Time-dependent transformations and off-Hugoniot processes
- New materials – discovery and applications
- Novel states of matter and new chemistry
- Deformation and transport properties of materials
- Liquids and amorphous materials
- New technologies and instrumentation

These topics summarize the current HP-CAT program while pointing the way to new capabilities and novel science, exploiting the new opportunities offered by the APS Upgrade and by the ongoing program of beamline technique development. It is noteworthy that the investigation of materials under extreme conditions is a major topic of the APS Upgrade, and hence that the HP-CAT programs are well in phase with the plans for the APS as a whole.

Phased upgrade program

The beamline management has developed a phased Upgrade plan, with Phase 1 currently underway (2012-2014); Phase 2 will follow (2014 – 2016), with Phase 3 scheduled for 2015/2016 – 2017. Phase 1 involves installation of a canted undulator, as well as time-resolved optics and advanced detectors. Phase 2 is synchronized with the APS Upgrade, leading to sub-micron probes and nanometer resolution X-ray imaging. For Phase 3, more work on advanced detectors is planned with further development programs on the imaging capabilities of the CAT (fast X-ray microscopy and tomography, and high-pressure coherent diffraction imaging.)

We find this phased program to be sensible and coherent, building on the experience and expertise of the beamline team, while exploiting the improvements brought about by the APS Upgrade (and employing APS expertise where necessary). The sub-micron focusing (a world first for a high pressure beamline) and nanometer resolution imaging will permit "next generation" experiments, including

- Even more extreme p-T conditions (towards the 10^4 K / TPa regime)
- More precise determinations
- Single-crystal experiments at the sub-micron level
- Grain boundary studies
- Combinatorial studies
- Composite materials

Technique development and sample environment

As mentioned above, a number of instrument/technique developments are planned for the next few years, continuing with the impressive program of equipment and technique development at HP-CAT. The result of this work over the last few years is a facility with exceptional integration of many different experimental techniques. The very successful laser-heating development will be continued, focusing on fast temperature changes to allow time-resolved studies. Single-crystal X-ray diffraction at high pressures is a very promising method. For time-resolved investigations the "white" beam Laué technique should allow studies of dislocations and deformations under pressure and stress. Another white beam method under development is very high speed radiography (up to 10,000 frames per second), used to study the dynamics of liquids at high pressures. For inelastic scattering a significantly smaller focus (5x5 μm^2 or even 1x1 μm^2) is planned.

The new science that will become possible depends to a large extent on the remarkable sample environment equipment made available by the beamline team. Sample

environment is a particular strength of this CAT. New work is planned in the three major areas, namely:

- Expanding capabilities in p, T and t (crysotats, diamond anvil cells(DAC), heated DACs, laser heating, dynamic pressure control)
- Sample preparation and probes (on- and off-line ruby systems and Raman systems)
- Increased efficiency of beamtime use (membrane and mechanical remote pressure control, on-line pressure measuring)

Taken overall, the CAT management and beamline staff have presented a coherent program of development over the next few years which is in phase with the planned APS Upgrade and should provide new scientific opportunities, while maintaining the CAT's position as one of the world's very best (if not the best) high pressure beamlines.

Staffing

Current staffing consists of 7 beamline scientists (100% funded), 3 beamline associates (100% funded), 3 support staff (100% funded), 3 postdocs (one 100% funded, and 2 others funded at 50% by the HPCAT operational fund). This yields effectively, 15 full time staff supported by the CAT.

Overall staffing was evaluated through discussions with staff both in a group setting, and privately, and by comparisons with staffing at other beamlines and CATS at APS and elsewhere. Although the staffing appears appropriate on a station/staff ratio basis, given the throughput of the beamlines, the number and complexity of the techniques that are supported, the amount of development in progress, and the aggressive nature of the coming upgrades, it appears the staffing may fall short of what is desirable.

Several staff members indicated they have heavy workloads and little time for their own intellectual and scientific development (in part due to HPCAT not providing staff priority research time). Others indicate that the demands of technique and software development place much stress on them, without elasticity in the organization to provide for this (e.g. with student or tech support, or acquisition of additional support staff). Not all staff had these concerns, but these considerations appear to have more significance at HPCAT than other CATs recently reviewed.

Staffing number and workload issues reflect an understandable tension between the need to drive relentlessly forward in the achievement of a world-class facility, and the individual needs of staff for a satisfying work environment that affords career-development potential. A challenge for HPCAT and for the APS in general is how to mitigate this tension for the good of all, so that significant numbers of staff are not disadvantaged. This is a crucial issue for the acquisition of new beamline scientific staffing, and for the ultimate encouragement of young scientists to enter such careers.

Adequacy of Funding

Funding for HPCAT has been consistent over the review period with a small increase. 75% of funds are derived from DOE-NNSA and 25% from DOE-BES, although post October 2012,

the 75% from NNSA comes directly via an agreement with CIW, whereas prior to this date the NNSA funding came via the three NNSA-supported partners (CDAC, UNLV, LLNL). The DOE-BES funding is via a separate grant to CIW. The principle issue with this support is that it is not diversified, and hence is subject to large potential changes. This is likely more a concern with the large block of NNSA funding. Given that the NNSA work is not subject to this review, and cannot be completely revealed, it is not possible to judge where this programmatic funding may be headed in longer term. As this is an appropriate concern for the APS as a whole, it is recommended that the management keep the APS informed about any potential changes in NNSA support well in advance.

Advisory Structure

The HPCAT scientific advisory committee, appointed by and holding meetings at the discretion of the HPCAT executive committee, advises on scientific plans, development feasibility, and enhancements of existing capabilities, at least in concept. However this committee has met only twice in the past four years, and does not appear to function with a purview or charge akin to the SAC for the APS, or as advisory groups do for other CATS. Current advisory members are C.C. Kao (SLAC), M. Rivers (CARS), W. Sturhahn (Caltech), M. Kunz (LBNL) and D. Shu (ANL). The role of this committee was discussed with several of the current members, who suggested it is not being used to advantage by HPCAT, or in a proactive way to address some of the challenges facing the facility. It would seem that a more regular meeting schedule for this committee, including significant charges and review, would benefit HPCAT, both in terms of addressing existing challenges, and also helping to remove the appearance that HPCAT largely operates without external oversight.

Self-identified ongoing challenges

Management identified several areas of significant challenges: Two major ones are software development and theoretical interconnection. Because of the large number of supported technologies, as well as their continuous development, and the workload of the staff, software development of user interfaces and analysis software often falls behind technical capability. This is a challenge for all APS CATS, but especially so for HPCAT due to the large number of different supported methodologies. The crux of the challenge is for management to decide how to allocate staffing to support the technical operation while keeping software development at pace. For unique staff scientists who have gifted programming skills, moving between these areas is facile. However in most cases specialists in software development are needed, and are much more efficient than staff not dedicated to such efforts. This is an area where close interaction and advice from the advisory committee could be very beneficial, especially in planning for the upgrade and resulting needs.

On the theoretical side the most likely enhancements might come from improvement and nurturing of increased connections with theoreticians working on materials or classes of phenomena being studied at HPCAT. This is another area where the advisory committee could be of great help, especially if appropriate theorists are added. An improved interconnection with theorists would be beneficial in support of present research

directions, but it would also be useful in identification of potential rich pathways for future investigations and technique/capability enhancements.

Other Challenges

We have indicated the challenges with staffing earlier, but another potential issue is the "insider" nature of the CDAC program. CDAC members are encouraged to submit proposals to the general user program, but also have a direct access route through the CDAC program to beamtime. It is not completely clear that this arrangement benefits the CDAC program or the general user program. On the one hand few CDAC members receive time in the general user program due to oversubscription and intense competition, so it is not clear that this affords useful experience to CDAC members, while it adds competition for "outside" general users. On the other hand CDAC members seem to have most of their needs serviced within the CDAC programmatic beamtime. It is in HPCATs best interest to contribute to a very strong and demonstrably open general user program at APS, and hence make available as much general access as possible. Hence for all these reasons CDAC application to general user time seems unwarranted.

An additional consideration is that individual staff research time, when not available during technique commissioning, is only available through staff application for general user time. This sets up a potential competition between general users, CDAC users and HPCAT staff for the same beamtime allocations.