

Summary Report of COMPRES Facilities Committee Meetings, December 15-16, 2015
Related to the COMPRES Executive Committee by M. Rivers December 18, 2015
Report submitted January 21, 2016

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The Facilities Committee met to review the annual reports submitted by the PIs of each COMPRES facility. Present were M. Rivers (Chair), A. Campbell, B. Chen, D. Shim, K. Lee, A. Kavner (Chair of Executive Committee), and C. Agee (President of COMPRES). The discussion continued among the committee members over two mornings. Summarized below are the issues that were discussed by the committee.

General points

It was agreed that in future years we should solicit information from each facility on user satisfaction. The synchrotron User Office should be collecting this information from end-of-run forms that each user group is asked to complete. This is definitely done at the APS, but we do not know if the ALS and NSLS-II collect this information.

ALS 12.2.2

The beamline continues to improve, and the management team is functioning well. The laser heating system is reported to be working well. COMPRES is leveraging considerable funding from the ALS. An improved setup for single crystal diffraction is being implemented with a high-precision diffractometer and a new CMOS detector.

Concerns

The fraction of publications related to Earth science is about 50%, which is consistent with the fraction of shifts that went to COMPRES users (51.5%). However, in the publications listed by Christine Beavers in her report only 1 out of 16 appears to be Earth science related. These are presumably publications that used single crystal diffraction. It was not clear if those publications were all from 12.2.2, or from other beamlines. Since COMPRES is supporting Beavers to develop single-crystal diffraction, it is important that it attracts COMPRES users.

The report from Jinyuan Yan was not as strong as that from Beavers. He lists a number of projects that he worked on, but with insufficient details to determine how successful they have been. How is the radial diffraction laser heating not working? What is the progress on the internal heating system? How many boron-kapton gaskets have been provided, etc. The committee was also concerned that he was a co-author on only one published paper during the reporting period.

There were concerns about radial diffraction with laser heating. 1. Separating high- T diffraction from surrounding cooler material is a major challenge. 2. At high T , the deviatoric strain is released.

Last year the COMPRES report said: “The Committee recommends that 12.2.2 staff keep better records of gas loading and laser mill users ...” The report this year did not include this information.

Recommendations

COMPRES is now supporting two stations that do single crystal diffraction, ALS 12.2.2 and PX² at APS beamline 13-BM-C. It is important that these groups coordinate to avoid duplication of effort and to provide complementary capabilities where appropriate. Users should be able to process data from either facility with the same set of software. We recommend that each facility provide a hands-on workshop for user training. Staff from 12.2.2 should visit PX², and vice-versa, either as part of these workshops or separately.

We were told by users of the facility that single crystal diffraction is only possible when Christine Beavers is present. We encourage the facility to train additional staff in this technique so that it can be used at times when Beavers is not available. We also understand that the Bruker analysis software requires processing data on-site unless the user has a license for the Bruker software at their home institution. We encourage the facility to provide alternative means to analyze the single-crystal data so that users can do it from their home institution with freely available software.

We recommend funding at the proposed level.

IXS at APS Beamline 3-ID

This facility continues to produce high-impact Earth science papers from this unique beamline. There were 10 published papers, plus one PhD thesis and 3 submitted papers. The COMPRES supported staff, Wenli Bi, has helped to organize workshops on Nuclear Resonance Scattering and High-Energy Resolution Inelastic X-Ray Scattering, and a symposium on Mössbauer spectroscopy, which are significant outreach efforts.

Concerns

The conventional Mossbauer is an important component of this facility, but it is not clear what publications, if any come from this, and which are from the online system. These should be broken out in the future.

Beamtime at 3-ID is very difficult to obtain because the beamline is heavily oversubscribed. In the Committee's request for the annual report from each beamline we provide a template file that asks for specific information, including the following:

- Total number of shifts requested
- Total number of shifts granted
- Total number of shifts available
- Oversubscription rate (= shifts requested / shifts available)
- Number of visits by distinct research groups

This report did not include any of the above information, so we did not have the information we need to know if COMPRES users are getting a fair share of the beam time. What fraction of the beamtime was requested by COMPRES users, what fraction did they receive, etc? We sent a request for this information during the AGU meeting, and the information is now available in the AnnualReport_Followup.pdf file.

The high-speed chopper is a major upgrade on the beamline, but there was no explanation of the capabilities it will provide and why it is useful.

Recommendations

We recommend funding at the proposed level.

Multi-anvil project at ASU

This facility continues to provide standard assemblies to many laboratories and to do new development for the community. They are now providing cell assemblies for the D-DIA at 6-BM. This year the developments included evaluating carbide cubes from different manufacturers and working on new pressure calibration standards.

Concerns

The Committee was concerned that this report was the first we learned of a project to evaluate carbide cubes from different manufacturers. While this is probably a worthwhile undertaking, in the future COMPRES management should be consulted before making a significant change in project scope. This change has resulted in an increase in the supplies budget from \$25K in year 4 to \$40K in year 5.

The assemblies that this project provides are enabling a lot of publications, but COMPRES is not getting credit for these. The PI should needs to provide a list of papers that have used the cell assemblies provided in this project. The Committee understands that a complete list is not feasible, but a list of at least 10 papers per year should not be very difficult to collect.

In the previous report for year 4 Tables 1 and 2 were much more informative. Table 1 listed all of the labs that had participated that year, and Table 2 listed the number of each assembly type that were provided that year. That information is lacking this year, so we cannot evaluate who is using the service and how many assemblies are being produced.

Recommendations

We recommend funding at the proposed level.

Carnegie IR

The COMPRES NSLS IR program was very successful, and the NSLS shutdown resulted in a loss of over 50% of the synchrotron IR capacity in the U.S. The program will move to the FIS beamline at NSLS-II where it will have 50% of the beam time, with the other 50% for the MET program.

Last year the plan was that FIS would begin operations in 2017. This has now been pushed back again until 2018 at the earliest, and that assumes the NSLS-II operations budget is fully funded. Until FIS begins operations the COMPRES supported beamline scientist, Zhenxian Liu is planning to run provide an offline facility for users using a conventional IR source at NSLS-II. He has also obtained a partner user program at ALS 1.4 with 10% of the beamtime. Liu has provided a microscope at this beamline for use with diamond anvil cells. COMPRES users are encouraged to submit ALS General User proposals, which if successful will be scheduled adjacent to Liu's PU time so that he can provide support for those experiments as well.

Concerns

The continued delay in the schedule start of operations at FIS is a serious concern. It now appears the dark period for this program will be at least 4 years, during which COMPRES is supporting a staff but has no beamline to operate.

The proposed user facility using the conventional source at NSLS-II has also been delayed due to the NSLS-II/BNL bureaucracy. From a technical perspective the system is ready to accept users, but there is not yet a Partner User agreement in place to allow this. The proposal submission process using the BNL PASS system, which would allow COMPRES users to get BNL badges to access the site, has also not yet been implemented.

They said they would announce the availability of the ALS 1.4 once COMPRES funding support was finalized. Does this mean the \$8,000 item in the budget for travel to ALS, or something else?

Recommendations

ALS may have a new IR beamline with a large dipole magnet opening angle, which would permit operations into the far IR. Liu proposes temporarily moving the new Vertex spectrometer there if that beamline is available much sooner than FIS. We support exploring this possibility.

Advertise the ALS 1.4 capabilities once it is officially running.

We recommend funding at the proposed level, including purchase of the new Vertex spectrometer.

We also agree with the recommendations from the COMPRES Site Visit Team report:

High priority: A reactive, quarterly work plan is needed for Zhenxian Liu. Because of uncertainties about COMPRES IR usage during the dark period, a detailed and evolving work plan will need to be developed during the offline period.

High priority: COMPRES leadership will follow-up and, as necessary, work with NSLS-II leadership to find a path forward for user access to an offline IR system as soon as possible.

Priority: Partner with Carnegie/Geophysical Lab for cost sharing during the interim period.

Priority: Advertise offline system and offline CO₂ laser heating system for users during dark time.

Priority: User interest should be monitored each year to confirm that COMPRES community members are using the high pressure IR facilities, both offline at NSLS-II and at ALS 1.4.2. It is hoped that community demand will remain strong, but if it is not then alternate staff deployments should be considered.

Suggestion: Perhaps establish a mail-in service to enhance use of the COMPRES IR facilities.

PX²

This facility has come online quickly. For the next run cycle (2016-1) 18 beam time proposals for 182 shifts were received through the APS GUP system. While 5 of these were from the University of Hawaii, the other 13 are from outside general users. PX² is supposed to receive 50% of the beamtime on 13-BM-C, which is 100 shifts in the 2016-1 cycle. The oversubscription is thus 1.8.

The beam size is 12 microns (horizontal) x 15 micron (vertical) with the new horizontal K/B focusing mirror that is collecting 2-3 times the flux as the previous temporary mirror system.

Concerns

While there were no publications from the experiments done so far, the committee hopes that publications will soon come from PX².

There was some worry on the committee that the large X-ray beam spot will make laser heating difficult. There was also concern about the single-sided laser heating design.

Recommendations

The committee feels that the top priority should be establishing a broad user base in the COMPRES community.

COMPRES is now supporting two stations that do single crystal diffraction, ALS 12.2.2 and PX² at APS beamline 13-BM-C. It is important that these groups coordinate to avoid duplication of effort and to provide complementary capabilities where appropriate. Users should be able to process data from either facility with the same set of software. We recommend that each facility provide a hands-on workshop for user training. Staff from 12.2.2 should visit PX², and vice-versa, either as part of these workshops or separately.

We recommend funding at the proposed level.

COMPTECH

The Technology Advisory Board is now functioning well, and is meeting on a regular basis to review COMPTECH progress and advise about future directions.

The work on thermal diffuse scattering has made substantial progress, and is potentially a new technique for deriving elasticity information at deep Earth conditions.

The project to provide a portable sample viewing system at sector 34 to allow this beamline to be used for diamond cell studies is excellent, and is exactly the type of project COMPTECH was originally envisioned to do.

Concerns

The COMPTECH technology officer Jin Zhang will be leaving to take a faculty position at University of New Mexico in the fall of 2016. This is the second time the person in this position has left since the project began. This is perhaps to be expected given that this is a soft money position of uncertain duration, but it has a significant impact on project continuity.

If a replacement for Jin Zhang is to be hired, will this person continue the TDS project, or will this be terminated because the new person lacks the interest or expertise to continue it?

There are a number of projects that COMPTECH is doing in addition to TDS: multigrain analysis, universal membrane cap, standard DAC heaters. Each should have a longer report so we can determine progress and problems.

We think it should be possible to implement the portable viewing system at sector 34 more rapidly than installation in September 2016.

It is not clear if this model of technology development is sustainable, or whether this role of technology development officer should move into the COMPRES central office with a higher profile and more stable funding. It is felt that the need for a technology officer responsible for facilities outside the APS is probably needed, including NSLS-II (e.g. for working on IXS and other beamlines) and perhaps at ALS (e.g. for expanding the IR program).

Recommendations

There was discussion about whether this program should be terminated when Jin leaves, or if a replacement should be sought to continue the program through year 5. In the end we decided that continuing the program is the best course until a longer-term solution for technology officer for COMPRES can be found, probably in the renewal proposal.

The replacement should be hired with several months of overlap with Jin to allow transfer of the programs and knowledge.

We recommend funding at the proposed level. We recommend that a search begin immediately for a replacement for Jin Zhang, which will allow for some period of overlap.

NSLS XPD and APS 6-BM

The multi-anvil and diamond cell programs at XPD were recently reviewed by a site visit committee composed of members of the Facilities Committee and the Executive Committee. For these programs we agree with the recommendations of that committee, and have only some updates to report. The APS 6-BM program was not reviewed as part of the site visit.

XPD Multi-anvil program

Concerns

The XPD program is now projected to start commissioning in September 2016, with first users in early 2017. This schedule has slipped by 15 months from the 2014 annual report from this group, which said that commissioning in XPD station D would begin in June 2015. Given the bureaucracy of NSLS-II with regards to documentation and safety the committee is concerned that this date could continue to slip.

For the multi-anvil program to ever expand at NSLS-II to have anything close to the amount of beamtime it had at NSLS will require a new beamline with a nearly dedicated station for the multi-anvil press. We have been told that proposed HEX beamline is such a potential location. However, the funding for HEX is from the State of New York with no mandate for high-pressure science, so it is not at all certain that even if HEX is built that it will be a home for this program.

Recommendations

We agree with all of the recommendations from the site visit report:

Highest Priority: A superb level of communication should be expected between the PIs of COMPRESS-supported diffraction programs at NSLS-II and COMPRES Central; this is an area where improvement needs to be made. This should include an integrated work plan for staff deployed both at NSLS-II and at APS.

Priority: Renegotiate a more advantageous partner user proposal with COMPRES as a co-signatory.

Recommendation: The XPD-MAP program should continue to be supported by COMPRES. Even at reduced PU time of 20% plus uncertain GU time, it will be important that highly competitive COMPRES-related MAP projects can be performed at COMPRES facilities. The user support for continued operation of a monochromatic X-ray MAP facility at NSLS-II is well established.

Since this program will have been without beam for over 2 years, but has continued to receive funding for supplies there is a considerable accumulated carryover of funds that can be used, so the funding for year 5 could be reduced from that requested.

XPD Diamond anvil cell program

The XPD diamond anvil cell program has been the subject of concern for COMPRES for several years. Last year the Executive Committee recommended terminating support for this program. The COMPRES PI for this program, Don Weidner, asked that this decision not be made without having a site review at NSLS-II. He also informed us that there was a pending NSF-MRI proposal that centered on the diamond anvil cell program. COMPRES conducted this site review in September 2015, and a report was produced and sent to the PIs of the NSLS-II projects for fact checking. The report was accepted by the Executive Committee in December 2015. We have subsequently learned that the NSF-MRI proposal was not funded, but that the NSLS-II will fund the K/B mirrors and electronics replacements that formed part of the MRI budget.

Recommendations

We agree with the recommendation from the site visit report:

The XPD-DAC program is the least well developed of the COMPRES facilities at NSLS-II, and is the one with the least COMPRES user endorsement. A more compelling scientific rationale for the DAC program is needed. At this stage it appears unlikely that the beam time proposals for the XPD-DAC program will be highly competitive for either GUP or PUA time. The science objectives articulated for the XPD-DAC program can be met at existing beamlines elsewhere, at which greater beam time commitments have been made toward high pressure research. Hence the Site Visit Team did not find cause to recommend overturning the Executive Committee's earlier decision to withdraw support for the DAC program at XPD.

The budget proposed for the DAC program in year 5 consists of \$83,850 for the beamline scientist, 45% fringe benefits and 26% indirect costs (total \$153,194). There is also about \$7,100 in diamonds and gasket material that is for the diamond cell program and \$3,600 for travel for this DAC staff member. These items can be deducted from the proposed budget.

APS 6-BM

The multi-anvil program at 6-BM has begun operations and has had its first general users. There were a few technical problems during this initial operations period, including a failure of the press stand during Shun Karato's beamtime, but things have been fixed.

Concerns

The committee was not sure why 4 hours per week of mechanical and electrical support were needed now that the equipment is installed and running. This comes to about \$44K per year, including \$6500 for riggers.

Would it make more sense for the multianvil users at 6-BM to use the user support laboratory at GSECARS, which is fully functional, rather than building their own?

The report said that "We clearly suffer from weaker beam than we had at X-17, but it is sufficient for most experiments". Is there quantitative information available on the measured difference in flux? X-17 and 6-BM are both about 30 meters from the source, so the flux through the same size slit should scale as the intensity (photons/s/0.1% bandwidth/mrad²) of the X17 superconducting wiggler and the APS bending magnet sources. These values are easy to compute, and the result is that X17 is 2.5 to 4.0 times more intense over the energy range of 20 to 100 keV. If they are seeing a greater intensity difference than this then something else must be wrong.

Recommendations

The facility is encouraged to solicit users to ensure full utilization of beamtime by as broad a COMPRES community as possible.

We recommend funding at the requested level with the possible exception of the shop charges mentioned above.

Sent request on Dec.21 asking why allocated beam time was only 57% of amount specified in Management Plan. This was answered in the AnnualReport_Followup.pdf file. The answer is that the time for 2015-2 and 2016-1 is as it should be, ~50% of the total time on the beamline for high-pressure.