

## **Summary Report of COMPRES Facilities Committee Meeting, December 13, 2016**

July 20, 2017

The Facilities Committee met to review the annual reports submitted by the PIs of each COMPRES facility (with the exception of the Gas Loading Facility at the APS which was reviewed by the EOID committee because of Rivers' conflict of interest).

Present were Mark Rivers (Chair), Bin Chen, Arianna Gleason, Anne Pommier, Dan Shim (Committee Members), Abby Kavner (Chair of Executive Committee), and Carl Agee (President of COMPRES),

Prior to the meeting each committee member prepared written comments on each proposal. Summarized below are the issues that were discussed by the committee in these comments and at the meeting.

### **General points**

It was agreed that in future years we should solicit information from each facility on user satisfaction. We were supposed to do so in 2016, but this was overlooked. 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 and the ALS. We do not know if NSLS-II is currently collecting this information.

### ALS 12.2.2

The report emphasized three main areas of new developments: single-crystal XRD system, external heating at HP, and two-sided laser-heated radial diffraction. The management team is functioning efficiently. The laser heating system is reported to be working well. COMPRES continues to do an excellent job leveraging considerable funding from the ALS. COMPRES-related users are reported to have large share of the overall beamtime (50-62%). The collaboration between beamline 12.2.2 with compressed-supported IR setup led by Zhenxian Liu is good use of resources, and is a unique capability. An improved setup for single crystal diffraction is being implemented with a high-precision diffractometer and a new CMOS detector. The COMPRES investment in a translation stage and collimator will be commissioned in the next 3 months.

The committee was pleased to learn that a student of Simon Parsons will be located at the ALS. This is a strong single-crystal diffraction group, and we welcome the collaboration.

The GSECARS gas loading system has been overbooked. Can beamline 12.2.2 pick up some of the load?

The external heating development sounds very good, but the committee is concerned that only users with BX90 cells can benefit from their capability. Does the beamline lend BX90 cells to users? How can it contribute to the broader COMPRES community?

#### *Concerns*

The fraction of publications related to Earth science is about 50%, but these appear to be the publications that the beamline management thinks are COMPRES related, they have omitted the ones that are definitely not. In the publications listed by Christine Beavers in her report only 1 out of 13 appears to be Earth science related. Since COMPRES is supporting Beavers to develop single-crystal diffraction, it is important that it attracts COMPRES users. It appears that there is only 1 single crystal high-pressure publication in the beamline publication list.

The report from Jinyuan Yan was not as strong as the one from Beavers and lacked care. Yan listed a number of projects that he worked on, but with insufficient details to determine how successful they have been. For instance, the committee wonders why the radial diffraction laser heating is not working? What is the progress on the internal heating system? How many boron-Kapton gaskets have been provided? The number of publications on which he is a co-author has increased from 1 last year to 4 published and 4 submitted this year, which is a nice improvement. It appears that he spends 5-6 days per month assisting users. This seems low, and questions were raised about Yan's productivity in the other 75% of his time.

#### *Recommendations*

For the last 2 years the COMPRES report said: "The Committee recommends that 12.2.2 staff keep better records of gas loading and laser mill users ..." The ALS 12.2.2 report this year again did not include this information and we strongly encourage the authors of the report to provide this information.

Last year we recommended that ALS 12.2.2 and PX<sup>2</sup> coordinate their efforts to be able to process each other's data, visits to the other facility, and workshops. The report does say that

they are developing export software so their data should be able to be processed with any “commercial” single crystal package. They also say they plan a workshop once the new ES1 station is complete. But there is no mention of interfacing with PX2 and thus, we recommend that a clear description of the efforts done to interact with PX<sup>2</sup> be added to the report.

This beamline has definite strengths and weaknesses compared to facilities at the APS. These should be clearly communicated to the user community, and we suggest that the facility should focus on experiments which play to their strengths, such as high-resolution studies with the mar345 detector.

The committee would like to have more information about the new \$200K detector. What station will it go on, and what are its characteristics?

## **IXS at APS Beamline 3-ID**

As it was the case last year, this facility continues to produce high-impact Earth science papers. There were 15 published papers, including 2 PhD theses in 2015-2016. The fraction of users with NSF-EAR support is high, which is excellent for COMPRES. There is a high acceptance rate for COMPRES proposals compared to general acceptance rate (70 and 47% vs. 30%). 25 grad students and 4 undergrads were involved in experiments. 40% of the available time goes to COMPRES users, which is much larger than COMPRES share of the total beamline support costs. 14 COMPRES user groups have been allocated beamtime in the past year. The report included excellent highlights on 4 selected Earth-related studies (velocity-density in inner core, core temperature, spin crossover in magnesio-wustite, iron isotopic fractionation). The committee appreciates that the report is very well written, and that it presents statistics for the offline Mossbauer system, which is something we asked them to do last year.

The COMPRES supported staff, Wenli Bi, again organized a workshop Nuclear Resonance Scattering. Dr. Bi also successfully conducted her own research and is actively developing high-pressure techniques for the COMPRES users. One PUP on "the low temperature and high-pressure NRIXS capability at sector 3" has ended, since it has reached its goals.

The committee is pleased to see that Sector 3 now has a Raman system for users. The planned and ongoing technical developments are well tuned for the Earth science and high pressure community. Most of the developments and upgrades are supported by APS.

### *Concerns*

The high-speed chopper is part of the "anticipated activities": is it not operational? Last year's committee report requested details about its usefulness, but this is still not addressed in this year's report.

The committee expressed concern about Wenli Bi's salary, which appears to be about \$70K/year, which is low compared to other COMPRES beamline scientists. A merit-based raise would be appropriate, considering the success of the program.

### *Recommendations*

Now that this facility is running the offline Raman system from GSECARS the committee would like to have statistics for this included in the annual report (how many users, how much Raman vs ruby fluorescence, etc.).

## **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. They are providing a large number of cell assemblies (3483) to the community, which is very impressive and demonstrates how useful this project is.

A new pressure gauge based on the (Ge, Si)O<sub>2</sub> and cohesive diffusion pair has been developed in collaboration with researchers at Sandvik Hyperion. The gauge is supplied to users free of charge. This is most useful for new labs to establish the pressure calibrations up to 10 GPa at high T. The development of the electrical conductivity assembly also appears to be quite successful.

### *Concerns*

COMPRES has funded the carbide development part of this project for 2 years, but there is no report on progress on this testing, just discussion of plans for the future.

The report includes 15 publications for 2015-2016, following last year's recommendation by the committee to provide a list of at least 10 papers, but this is still clearly far from a complete list.

### *Recommendations*

We recommend that the PI work to ensure that all publications that result from the use of the cell assemblies include a standard acknowledgment of COMPRES support, and that the PI be informed of all publications that used the cell assemblies. A document with this requirement should be included with each shipment.

The committee recommends that in the future the report should break down the publications by category: those resulting from the development projects, and the science papers resulting from the cell assemblies they provide to users.

## **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.

Significant progress has been made in the commissioning of the IR beamline at NSLS-II. The report listed the planned activities with adequate funding from NSLS-II and clear time lines. The NSLS-II has issued the purchase orders for the FIS/MET experimental stations, and for the IR extraction port on the storage ring. These are both very welcome, and provide reason to hope that there will indeed be IR beam at NSLS-II in 2018, 4 years after the shutdown of NSLS.

To bridge the gap between NSLS-I and II, an offline IR system has been set up and is now accepting user proposals. Almost 30 user proposals have been allocated laboratory time. This partly reflects the user base of the upcoming IR beamline at NSLS-II. The mail-in service appears to be quite successful. The user base and science output are well documented.

The temporary IR setup at 1.4.3 beamline of ALS seems to be a good solution for the "dark" period.

### *Concerns*

There is very little information about the program at the ALS. Last year we said:

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.  
There is no update on these items.

One of the committee members found that the XRD+IR combination that ALS can offer is very useful, facilitating the conduct of unique experiments.

- However, the beamline scientists at 1.4.4 were unsure about retention of the system installed there after NSLS-II comes online. Their impression was that the system will eventually return to the East coast.
- The IR system installed there works OK but appears to be installed temporarily. The system is installed on a thin aluminum breadboard which is very unstable. With small investments the system could be much more stable and user friendly.

The committee appreciates that scientific highlights are well-written and show new results on perovskite, structure of zeolite, molecular bonds, and nanotubes. However, most of the work is not related to Earth Sciences, and it seems that a lot of non-Earth science work is supported by COMPRES (as mentioned last year in the committee's report).

### *Recommendations*

The committee recommends advertising the ALS 1.4 capabilities (a recommendation that was also made last year).

The following were the recommendations from the 2015 COMPRES Site Visit Team report, along with the current status:

**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.

**Not completed. Please provide a detailed work plan for Liu.**

**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.

**Completed.**

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

**Not completed. Carnegie is no longer the PI's home institution.**

**Priority:** Advertise offline system and offline CO<sub>2</sub> laser heating system for users during dark time.

**Not mentioned in report, so the committee does not know the status. Please explain.**

**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.

**The use of the offline facility is documented, but the usage of the ALS is not. Please explain.**

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

## PX<sup>2</sup>

PX<sup>2</sup> continues to progress quite well. Clear scientific highlights underline new results relevant to Earth sciences, such as phase equilibria in the Fe-O-H system, and investigations of high-pressure phases possibly present in subduction zones (omphacite, pyroxenes). Beamline developments and planned work are in excellent agreement with the user community needs. A broad user base has been developed in the COMPRES community, and COMPRES members get >77% of total beamtime granted under this program.

6 publications are reported, including 5 on high-pressure single-crystal diffraction, compared to no publication last year. One of these is a high-profile Nature paper. The committee notes that there is only 1 on high-pressure single-crystal diffraction publication from ALS 12.2.2 which has been running single-crystal for longer.

45 beamtime requests were received, compared to 22 in 2015, which shows good improvement.

Przemek Dera is investing in the facility outside of COMPRES by stationing 2 students on year-long stays at the APS doing single-crystal studies.

### *Concerns*

Last year we said the following:

COMPRES is now supporting two stations that do single crystal diffraction, ALS 12.2.2 and PX<sup>2</sup> 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 PX<sup>2</sup>, and vice-versa, either as part of these workshops or separately.

This is not addressed at all in this report.

The report did not mention the plans for laser heating, but the laser is already present and there should be a plan for integrating it. There was concern last year about the design of the single-sided laser heating system, and this was not addressed in the report.

### *Recommendations*

The committee recommends continuing the expansion of the COMPRES user base.

The project must address coordination with the ALS single-crystal program.

The project should report progress on the laser heating system.

Last year's committee report recommended that PX<sup>2</sup> and ALS 12.2.2 provide a hands-on workshop for user training. It seems that this has not been done yet; therefore, the committee renews this recommendation.



## COMPTECH

This is a “close-out” report for the COMPTECH project which has been discontinued. The committee appreciates Przemek’s comments on the lessons learned from COMPTECH.

### *Concerns*

The publications listed in the COMPTECH section of the combined PX2/COMPTECH publication list are actually all unrelated to any COMPTECH projects. They are Jin Zhang’s research on other projects.

The committee wonders if there is any mechanism to continue the excellent work on DAC membranes, DAC heaters, and portable ruby fluorescence systems.

### *Recommendations*

Last year, the committee report said:

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).

The committee continues to think that COMPRES should consider having a position for a “technology” support person at a higher level. One of the strengths of GSECARS and HP-CAT has been that they have the technical staff and expertise to design and construct equipment for new techniques. COMPRES really does not have this, and it could be very useful.

In the first COMPTECH project a Web site with very useful links for software and data analysis was prepared (<http://comptech.compres.us>). This should be taken over by COMPRES central, and kept up to date. Modules on training would be very helpful. COMPRES central can maintain the site, but others need to contribute the content.

## **NSLS XPD Multi-anvil program**

The science highlights from Karato, Raterron, and Hunt are all very exciting and well-written. However, these are nearly all based on experiments conducted at the old NSLS which ceased to operate in 2014, and in fact some of the publications themselves are from 2014 and do not belong in this report.

### *Concerns*

The progress on XPD continues to be slow, and the committee understands and shares the frustration of the facility members. While partial blame is put on the COMPRES PU not being completed, the committee would point out that this was only a recent problem, and thus, it does not explain why this facility is now nearly 2 years behind what was forecast in the 2014 annual report, i.e. commissioning with beam in June 2015. The committee is aware that part of this issue is certainly the increased red tape and regulations of NSLS-II, but also that the Stony Brook management may share some responsibility. The Delta Tau controllers are in use around the NSLS-II, and also at GSECARS. These groups have experience in controlling them from EPICS, and certainly GSECARS would be happy to assist the XPD MAP project with this, but they have not asked for help and are still struggling on their own. The fact that the Delta Tau controllers came without power cords seems unfortunately to be due to mistakes in the purchasing planning, since GSECARS did not have this problem when they received their units.

In the report, the delays are attributed to the cancellation of the DAC part of XPD, mentioning that they had to go “back to the drawing board”, with no explanation of what they actually had to do because of this decision. The DAC and MAP were quite separate, and the committee does not understand this comment.

The issue of how a DT25 to work with monochromatic beam will be built is an important one, and the committee regrets that only 1 brief paragraph was dedicated to it. The committee understands that a solution does not exist yet, but there are “still have a few (geometries) to try” and more information about them would have been welcome.

The committee appreciates the fairly detailed list of tasks that need to be done to for technical commissioning in 2017-1. A timeline with dates so that they can evaluate their progress should be added. They need to have a timeline that NSLS-II agrees to.

The committee thinks that some of the activities they list for 2017-2, like design of a temperature measurement system could begin immediately.

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.

The report by M. Whitaker lacks details and statistics and is in a CV format. His report listed some workshops, but it is difficult to tell whether he organized the workshops or just attended them.

### *Recommendations*

The project needs to produce a clear project timeline which is agreed to by NSLS-II. The committee is very concerned that if this is not done immediately the project milestones will continue to slip. COMPRES management needs to closely monitor the project progress, perhaps with monthly status reports and phone calls.

The committee recommends that COMPRES and Stony Brook negotiate a final Partner User Agreement with NSLS-II as soon as possible. If the fraction of beam time for the multi-anvil program is less than the currently agreed 20% then COMPRES needs to know this for future planning.

### **APS 6-BM**

The report focuses on the full year operation of the beamline 6BM at APS. The 6BM beamline has served 32 unique users and appears to be in demand for studies on the rheology of the deep Earth.

#### *Concerns*

The committee thinks that the quality of many of the proposals getting beam time on this beamline is not as high as we would like to see.

The report on the ultrasonic system has not been updated, and still refers to the system being “fully integrated on X17B2”. It has actually run on 6BM, but there is no mention of this in the report.

There is no detail about the science presented in the report of Chen.

Both Chen and Whitaker (100% COMPRES support) are both heavily involved in the development and maintenance of the instruments and participate in research but are not included in very many publications. The committee thinks that there is a lack of recognition for their efforts. Also, it is unclear if Chen is involved in any NSF proposal (not listed), and all the proposals of Whitaker as lead PI have been declined; is this something that could be improved? (such as having more time for proposal co-writing?)

#### *Recommendations*

The committee recommends that the facility improve its outreach to solicit users to ensure full utilization of beamtime by as broad a COMPRES community as possible.

The future of 6BM should be left open until XPD begins to operate and we can assess the relative strengths of the two programs.