02.07.2014

ALBA Scientific Advisory Committee

18th Meeting held on
July 1st – 2nd 2014 at ALBA, Barcelona / Spain

ALBA SAC members present:

Oliver Bunk, PSI, Switzerland
Andrew Fitch, ESRF, France
Peter Guttmann, HZB, Germany
John Helliwell (Chair), Manchester University, UK
Andreas Jankowiak, HZB, Germany
Nick Terrill, DIAMOND, UK

ALBA SAC members not present:

Amor Nadji, SOLEIL, France
Jose Enrique Ortega, University of the Basque Country San Sebastian, Spain
Sakura Pascarelli, ESRF, France
Ian Robinson, London Centre for Nanotechnology, UK

1. Introduction

The 18th Meeting of the Scientific Advisory Committee has been held at ALBA on 1-2 July 2014. The sections below have been provided by specific individuals of those present at the SAC18 and collectively discussed at the SAC18. Subsequently, in the two weeks after the SAC18, Members had the opportunity to offer corrections and suggestions to the Chairman.

2. Safety

We greatly appreciate the high effort made by the management to simplify the safety issues for user access as much as possible. Additionally, the discussions lead obviously to clear statements about the responsibility of a beamline scientist regarding safety issues. From the user feedback forms (up to the end of 2013) only a few complaints about the procedure are visible. We encourage the management to continue in their efforts.

3. User feedback

Comments

The user feedback on the beamtime is a potentially valuable tool. It could be helpful to exchange experience with other facilities both regarding the procedure for getting feedback and the interpretation of it. Low statistics, i.e., low return rates are observed at other facilities as well. In general one should assume that no feedback means that the users are satisfied, i.e., had neither extreme problems nor were extremely satisfied. Personal feedback close to the end of an experiment is not replaced by the web-questionnaire and if provided, very valuable for the beamline staff to recognize and discuss specific issues.

Recommendations

The feedback should be provided promptly to the beamline scientists as soon as the users provided it. An online tool where the beamline scientists can retrieve the feedback whenever they want will be helpful.

The feedback should be provided by one principal investigator per experiment rather than by each user. This will reduce diversity of the results and help interpreting them.

The feedback must not be anonymous, i.e., it must be directly linked to an experiment number and title. Of course principal investigators should be aware of their feedback being passed on together with their name to the local staff. Established in this way the beamline staff has a chance to follow up on extreme ratings and comments to get more details. Typically this is appreciated by users at other facilities, i.e., it is advantageous for both users and local staff if the feedback is not anonymous.

It will be helpful to establish a follow-up procedure in all cases where 'poor' ratings are given; the beamline team can ask the principal investigator for more details. Often this will resolve the issue and the rating alone turns out to be not adequate.

Local contacts should be encouraged to ask explicitly close to the end of a beamtime for feedback from the users. Personal discussions render this feedback very valuable.

4. ALBA data preservation policy is needed

Expectations of Governments for the preservation of scientific data, paid for by tax payers, are increasing. For ALBA this can be via the Facility (eg the Australian Synchrotron and ARC method ´TARDIS´) or via the PIs as Users of ALBA (and their home universities) but

clarity of who is responsible for the long term preservation of scientific raw data measured at ALBA is essential. Scientific data that does not lead to a publication after a Government defined period increasingly is expected to be accessible by the public (ie including other users) to analyse and publish about. Appropriate metadata have to accompany all such data. Besides Australia´s ´TARDIS´ another exemplary effort is at ISIS. An overview report from IUCr (and other relevant reports from ICSU/CODATA etc) can be found at the IUCr´s Forum ´´Public input on diffraction data deposition´´:-

http://forums.iucr.org/viewtopic.php?f=21&t=343

5. Overall technical comment across all beamlines

Thermal drifts and the need for improved air conditioning were a reoccurring theme across many of the beamline presentations. To give an example, day-night cycles of the temperature in the meanwhile air conditioned XALOC hutch are likely causing drifts of more than the size of the focused beam and are likely introduced by day-night cycles from the hall temperature. Such effects should be recognized, their reason should be understood and they should be fixed. For this purpose it would be helpful to have data on the stability of the air-temperature over day-night cycles:

- in the storage ring tunnel
- in the experimental hall, e.g., close to soft X-ray end stations
- in the optics hutches
- in the experimental hutches

The overall responsibility for addressing these temperature stability issues should be clear.

6. Format of the meeting

A lunch-to-lunch format with a more focused selection of topics would it make it easier for some members of the committee to spare the time for attending the meeting. Such a format is successfully used at other facilities. Talks focusing on a single beamline are compatible with this scheme, if one switches to reporting each year or each one and a half years for individual beamlines. It might be helpful to schedule the time for talks and the time for questions regarding the talks separately. This helps speakers in preparing a presentation of the desired length and assists during the meeting in reserving sufficient time for discussions and thereby feedback.

7. Industry

Findings

The Industrial office reports its

- VISION: Contributing to improve the Industry competitiveness by using the latest Synchrotron Light developments.

- MISSION: To promote and to make available to the Industry all the potential of the Synchrotron Light applications.
- STRATEGY: Customer satisfaction, one-stop shop service
- ORGANIZATION: Office reporting to the Director staffed by two persons

The industry focus at ALBA has been in operation for one year so far. The group deal with both Industrial User access and collaborations to design/build equipment. They are engaged in Outreach activities which will be key to developing this side of the ALBA operations. The team realise that analysis was key to helping Industrial users although understood that the breadth of expertise in the Industrial community was likely to be as broad as that in the Academic one. Currently Beamline staff are essential to this with no plan currently to employ scientists in the Industry Group.

ALBA are already actively pursuing Technology Transfer where collaborations are being set up to spin out technology developed at ALBA. This is to be commended.

Comments

The spread of industrial use at ALBA seems different to other synchrotrons but this may be down to the model for many Pharmaceutical companies here where they outsource their purification and crystallisation effort. This should certainly be followed up as this field is where many other facilities bring in most of their Industrial revenue. It was felt that the other gap, Non Crystalline Diffraction, would grow as the industry effort grew.

There is, as yet, no policy for allocating Industry time as there is too little of it to worry about and there are currently plenty of gaps in the scheduled as beamlines work towards steady state operation. It would be good to have something in place before they reach this so everyone is clear as to how the industry work is going to be operated.

There is at present no target set by Management for the total Industry time expected or to be aimed at. As the policy on Industry develops it would be useful if this subject was discussed both internally and with stakeholders so everyone was clear as to what the goals were.

Currently beamline staff are expected, as the acknowledged experts, to actively participate in all industry time on their beamlines. While the level of Industry take up is low this model is OK but if, as one would hope, the industrial work increases serious thought should be given to using the Industry revenue to recruit dedicated staff to carry out this necessary work, so as not to overburden the beamline staff and detract them from developing their beamlines and their own science activities. An alternative used in some places would be to incentivise the beamline teams to carry out the Industrial work with funds being assigned to beamlines that carry out industrial contracts but this still carries the work burden discussed above.

Several models for how industrial work is carried out exist and only time will tell which will be of most value to ALBA. First and foremost getting Industry in is important, as long as the beamline team feels the beamline is ready. The quickest way to alienating Industry is to say yes and then not produce good data that can be analyzed easily. It is also important, if you are going to do the full analysis, to only do work where there is expertise at the facility. This might sound obvious but if the field is outside the expertise of the team then it can be a major drain on resource and mitigates against having the industry money in the first place.

8. Machine Status and Top-Up Operation

Findings

Francis Perez gave a comprehensive overview of the accelerator operation and developments of the years 2013 to mid 2014. Due to problems with the cooling system and an vacuum incident 1416 h of operation were lost, from which 824 h could be recovered by rescheduling. A total of 2971 h had been delivered to the users. Without accounting the above mentioned major incidents, the average availibity reaches 96.2 % with an MBTF of 25 h and 0.8 h time to recover. These values increases to well above 97 % availability and 40h MBTF for the first half of 2014, whereas the recovery time is still in the order of 1 h per incident. These numbers are already well in the ballpark of the other 3rd generation light sources and clearly shows that ALBA is on track, still with room for further improvements.

To guarantee the longterm availability of the machine, 5 IOTs of a new manufacturer (L3) have been order as replacement spare parts for the 500 MHz high power transmitters, due to be delivered 2014/2015. The waveguide system of the linac had been modified by integrating waveguide switches to be able to operate, with a somewhat reduced energy of 67 MeV, with only one of the two klystrons in case that one fails. At this lower energy beam emittance and energy spread is increased by a factor of 2.

Following lots of preparatory work, from 25th to 28th of June first TopUp operation with users at the by now standard value of stored beam current of 120mA take place. The beam current had been stabilised to the order of 1mA by injecting approx. each 20min, a scheme which all beamline responsibles had agreed on. The measured radiation levels in the hall were well below the legal values and in the order of 40% of the TopUp permit level. Except BL24, all beamlines reports that their measurements are not affected by the injection process. The problem at BL24 will be solved by making use of the gating signal provided for TopUp injections. Operation of the 3Hz booster power supplies (starting 3min before injection takes place) is accompanied by some uncomfortable noise at 12.5 KHz on the experimental floor; technical measures are underway to reduce it to an acceptable level.

Very successful first tests of Fast-Orbit-Feedback (FOFB) had been reported, showing a nice reduction of beam noise up to frequencies of 100 Hz. Aside these major efforts, many other improvements took place. E.g. a tool has been set-up which improves the closure of the injection kicker bump by analysing turn-by-turn BPM data (important for smooth TopUp injections). Beam energy measurements done by spin depolarisation measurements shows a day-by-day stability of well below 10^{-4}. Importantly, a tool had been set up, which allows to calculate a modell based beam life time from measured beam parameters. This is an important measure to optimize beam operation, especially under TopUp conditions. Up to now some of the underlying parameters of this “lifetime calculator” are still adjusted “by hand” to fit to the measured beam lifetime. Clearly further effort is necessary to establish a clear view on the different processes determining the overall beam life time.

SAC congratulates the ALBA team for the excellent progress achieved during the last year.

Comments

- A reliable metrics, which allows comparison with other facilities, is important for the long-term analysis of the performance of ALBA in terms of reliability and availability.

SAC encourages ALBA to follow the path, as already started, of applying a standardised metric for all light sources as proposed on IPAC14.

- To reduce the probability of further pin-hole like "water spray leaks" due to cavitation in small diameter piping's, ALBA should take care, that the water flow is carefully adjusted to be reasonable above the minimum flow level defined by the interlocks, but not being to excessive, as cavitation is a process which abruptly starts when exceeding a certain flow speed.
- Purchasing spare IOTs of a different manufacturer (L3) is a very reasonable measure to guarantee the availability of ALBA and secure the large investments done for the RF transmitter stations. It may be worthwhile to start acquiring first experiences and expertise with solid state amplifier transmitter stations on a longer time scale by replacing the booster transmitter station. But this is clearly not a urgent need.
- The radiation level under TopUp conditions is determined by the average losses due to finite beam lifetime and the injection efficiency. In total these losses are proportional to the average beam current divided by lifetime and divided by the injection efficieny. With increasing beam current, the radiation level will certainly increase due to the higher average losses and therefore it will become more and more important to guarantee an injection efficiency above a certain level. ALBA should carefully track the development of injection efficiency, understand how to improve and to maintain it on a high level. Exceeding 80% efficiency on average should be the goal for the future.
- Apparently there seems to be no need for special filling patterns (like camshaft bunches). Nevertheless ALBA should be prepared and further explore and develop the single bunch capabilities of the injector chain. This would also provide more flexibility for TopUp operation. In this context it should also be checked, if the emittance at the end of the acceleration process of the booster is still somewhat influenced by the linac emittance, as this could affect injection efficiency when operating with reduced linac energy.

Recommendations

- SAC strongly recommends to establish TopUp as standard user operation as soon as possible. Everything from the machine side seems to be well prepared and long term experience to optimise all procedures can only be gained in user operation.
- The detailed TopUp scheme (current to be refilled, time interval between injection) should be regularly revisited together with the beamline responsibles.
- Any substantial increase in beam current, which above certain levels needs to be accompanied by other measures like establishing bunch by bunch feedback, will certainly change the TopUp scheme.
- SAC also recommends to establish FOFB for standard user operation as soon as a reliable operation is possible. Only FOFB in combination with TopUp will provide the basis for highest beam stability and increase operational headroom to cope with unexpected noise acting on the beam.

9. Phase II Beamline process

Comments on feasibility of proposed schedule and objectives:

MIRAS

- Positive synergy ALBA-user community in the starting design of the beamline and posterior development being done in-house.
- Big effort of ALBA human resources acting as project management.
- The beamline responsible should join the final development of the beamline as soon as possible.
- Realistic proposed schedule: Construction completed within 2015 and first users expected in 2016.

LOREA

- The good communication between ALBA management and user community involved in the beamline proposal should continue.
- The new beamline scientist staff already approved should be incorporated as soon as possible in order to increase human resources for carrying out the proposed schedule.
- It is feasible to have the first users in 2018.

10. Report on BL MSPD

- **Scientific and technical weakness and strength**

The beamline has an able and committed scientific team that understands fully the opportunities offered by the beamline and the needs of the scientific user community. The beamline offers excellent capabilities in high resolution powder diffraction, in-situ studies, PDF analysis, and high pressure diffraction, and is competitive with high quality facilities at other SR sources. There is a good balance between the use of the various techniques and a large user community. Papers in quality journals are beginning to flow. Industrial activity and interest are developing well.

- **Identify critical path if any**

Powder diffraction is a technique that relies heavily on the provision of sample environments. The SAC is pleased to see the acquisition of a cryostat; however, it is important that sufficient resources are available to continue the expansion of sample-environment options, as required by the developing user program. Careful co-ordination with CLAESS for shared equipment will be necessary.

- **Are there missing scientific fields where ALBA should focus with the available techniques/hardware?**

Powder diffraction is a flexible technique that can adapt readily to a wide range of scientific areas (e.g. we note the recent strain-mapping experiments). Technical resources for the (usually) modest technical requirements should be available.

- **Comments on postponing BL technical reviews until 3-4 years of operation**

The SAC would support this for MSPD; the beamline infrastructure is clearly producing high quality science, and allowing the program to reach a certain level of maturity before review would seem appropriate.

11. Report on BL MISTRAL

- **Scientific and technical weakness and strength**

Mistral is now in full user operation and first results are presented.

One high impact publication and a very recent thesis underline the quality of Mistral for biological applications. Additionally, good work in materials science can be measured by it being awarded a "best experiment" namely that entitled "imaging magnetic domains at Mistral".

It has to be noted, that due to the complicated setup (similar situation for high-end TEMs) nearly all experiments need a full time support by the beamline staff. Only long term users can be trained to operate the microscope.

The ongoing technical developments (incorporation of a fluorescence light microscope, development of online data analysis software, evaluation of spectroscopy at the carbon edge) will improve the strength of Mistral.

- **Identify critical path if any**

Due to the full time support for user experiments including adapting Mistral for their specific needs time for necessary developments seems to be quite restricted.

Data processing needs fast computer systems with highly available memory and storage capacity.

Long term data archiving is not solved.

- **Are there missing scientific fields where ALBA should focus with the available techniques/hardware?**

No

- **Specific recommendations in case of identified common weakness or problems.**

The top up tests should be continued under realistic working conditions, i.e. with wobbling condenser, to clarify if there is an impact on the image quality and photon intensity.

The stability of the illuminating beam should be higher in top up mode. More detailed commissioning on this has to be done.

There should be some dedicated commissioning beam time for spectroscopic developments.

So far, 300 mA beam current seems to be not necessary for Mistral.

Long term data archiving of user data (10 years?), which data – only raw data? These issues should be discussed. Additionally, it has to be discussed if full data analysis for users should be made available on the IT structure of ALBA for users. Are there any plans regarding the European PaNDAas initiative (i.e. as the successor to PaNData)?

- **Comments on postponing BL technical reviews until 3-4 years of operation**

Results from one user run are normally not enough for a publication in X-ray microscopy. Typically, several runs are necessary to consolidate results. Therefore, it is recommended to postpone the technical review.

- **Comments on post-docs poster session**

For spectroscopy applications re-alignment and calibration of the monochromator needs to be done.

12. Report on BL11-NCD

There has been a lot of work put in to improve this beamline since the last SAC meeting. The team are to be commended on this and it is good to see that calibrations so energy selection is smooth are now in place. The SAC is glad to see progress on ImXPAD. Even if not installed finally on beamline, it is good to see progress here as this was one of SAC's major concerns at the last meeting.

The data presented from the factory acceptance tests had some flaws but SAC was informed that these would be replaced before final installation. There have been some compromises on the ultimate speed performance but these should not impede the use of the detector for much of the science likely to be carried out on BL11. The Instrument Responsible informed SAC that the ADSC will still be used regularly for slower experiments. This is a pragmatic view given the active area of the ImXPAD. This is a good detector but its excellence should not be overplayed as it is comparable to other options available.

SAC does have a couple of questions which the ALBA management should consider for the detector.

1. What is the support contract for the detector going forward? It is worrying that the company has not even an X-ray tube for testing.
2. Will effort from the company be available to improve performance to the original Ultimate Specification?

The software is being developed too, pyFAI being used for calibration for example. There is a good range of in house science and it is clear that the beamline is settling down into operations as the publication record is starting to improve.

There are still some areas that need addressing as evidenced by the extensive upgrade programme which reads almost like a rebuild, however SAC is concerned that the KB upgrade was at the bottom of this list and, as yet, not approved. Variable focus for a SAXS beamline is essential if it is to perform well and meet the needs of its user community. The down time described to change camera lengths is just not acceptable when other facilities can carry out this task in 1hr or less. Temperature stability is also essential for both hutches and as was seen in other talks ALBA should consider this as a priority now the machine is running top up so the beamlines can take full advantage. It would be interesting to SAC to see how ALBA views the spread of science between Life Science and Physical Science developing as this would dictate other advice. For example, if BioSAXS is to be a major strand some level of automated delivery system would be essential for BL11 to compete in this field across Eu-

rope. This is missing from the upgrade project list and should not be if funds are not available to purchase the EMBL designed BioSAXS robot. A project of this size will take time and should be started as soon as possible as SAC notes several of the beamline teams own science areas would require one.

On the whole users seem very satisfied with the beamline and some of the User complaints maybe more a user education issue than any real problem.

13. Report on BL CLAESS

- **Scientific and technical weakness and strength**

The beamline has made significant progress, with a vigorous new scientific team, and is finally operational with users, producing high quality science. Papers in recognized high impact journals have been published. The extension of the operating range towards70 keV is a commendable development, opening up opportunities not foreseen in the original specification of the beamline. There is an increasing level of industrial use.

- **Identify critical path if any**

The SAC is happy to see that the CLEAR spectrometer has been installed, and supports the proposed commissioning and development timetable, with user operation in mid-2015. This device will give the beamline unique capabilities.

- **Are there missing scientific fields where ALBA should focus with the available techniques/hardware?**

The range of scientific fields is appropriate for now, with emphasis on catalysis, solid-state physics, cultural and environmental issues, etc. The beamline should evolve as user demand indicates; absorption spectroscopy is generally a flexible technique that can adapt to a wide range of disciplines.

- **Specific recommendations in case of identified common weakness or problems.**

Sharing of equipment with MSPD should be carefully coordinated. The gas flow system and the mass-flow controllers could become a problem if they need regularly to be transferred between the two beamlines.

- **Comments on postponing BL technical reviews until 3-4 years of operation**

This would be appropriate to allow the capabilities of the CLEAR spectrometer to be realized.

14. Report on BL CIRCE

Findings

The beamline is in user operation with the PEEM and early user operation with the NAPP end station. Good results are shown for the PEEM. The NAPP just passed the site acceptance test.

The urgent issues with the Irelec KB motors have been successfully addressed. The delicate task of carbon cleaning from the high-energy grating is in progress.

Top-up mode tests yielded the expected result of no effect on the position but drops in intensity during the top-up injections.

The oversubscription is high due to the combination of a large number of proposals and a 'typical' beamtime requested being on the order of one week. Currently the number of in-house and user publications is still marginal.

Comments

Experiments performed at CIRCE might often require more than one beamtime for a positive outcome that is reported in a publication. The intense support and habits in the community will likely lead to most user publications being co-authored by the local contact at the beamline. This is positive for the local staff but adds at the same time the burden of following up on each experiment.

Setting priorities between commissioning further equipment and operation modes and bringing past experiments towards publication is an delicate issue.

The planned implementation of continuous scans might improve the scientific productivity of the beamline.

The observed intensity drops during top-up injections are likely to be considerably reduced after optimizing the top-up operation and the FOFB in user operation.

Recommendations

We encourage the beamline staff to further optimize the beamline for top-up mode with FOFB in place. An exchange of experiences with other facilities that use top-up mode for similar experiments should be considered.

For further optimizing the beamline the team should define 1-2 high-priority experiments together with 'power users'. These define the priorities in further commissioning the various components and the team should be involved in the further data analysis and writing of the publications.

15. Report on BL BOREAS

Findings

The beamline covers the energy range from 150 to above 2000 eV at high flux and 80-150 and from 2 to slightly beyond 4 keV at lower flux.

The HECTOR end station provides good temperature (2-350K) and magnetic field (6T along beam) range for XMCD measurements and is in user operation since May 2012. The MARES end station, a magnetic scattering reflectometer, is planned to go into user operation in spring 2015.

Implementing continuous scans greatly benefits experiments both qualitatively and quantitatively.

Urgent issues like leaks and the replacement of damaged motors are successfully addressed.

First publications appear in well-established journals for the field.

Comments

Covering the 2000 – 4000 eV range, even at reduced flux, opens up options for experiments that cannot be performed at many other facilities. This may be utilized more once both end stations are in regular user operation for some time.

Debugging and further development of beamline control software requires a close collaboration between the controls and beamline team.

Experiments performed at BOREAS might often require more than one beamtime for a positive outcome that is reported in a publication.

The intense support and habits in the community will likely lead to most user publications being co-authored by the local contact at the beamline. This renders the publication of a 'beamline paper' less urgent.

Recommendations

We encourage beamline and machine group to further commission top-up mode with FOFB and to benefit from an exchange of experiences with other facilities that use top-up mode for similar experiments.

For commissioning MARES the team should define an in-house or 'power user' day-1 and year-1 experiment. These define the priorities in commissioning the various components.

16. Report on BL XALOC

- **Scientific and technical weakness and strength**

- Overnight usage could be improved;
- To objectively assess ´strength´ could compare with similar maturity MX beamlines via BioSync website e.g. how does xaloc PDB depositions compare with Shanghai MX BL?

- **Identify critical path if any**

Good suggestions from in house re planned developments

- **Are there missing scientific fields where ALBA should focus with the available techniques/hardware?**

No

- **Specific recommendations in case of identified common weakness or problems.**

The likely positive impact of top up needs to be dissected out by looking at short term rms source position fluctuations as distinct from long term i.e. diurnal temperature variations.

- **Comments on postponing BL technical reviews until 3-4 years of operation**

No comment at present

- **Comments on post-docs poster session**

A good idea.

17. Phase III Beamlines process

The phase III Beamline process has been discussed, the evaluation criteria defined. They are listed in the Annex, which corresponds to the final version defined few weeks after the SAC meeting.

18. Summary of main recommendations from SAC 18 arose from:-

- Top up and FOFB clearly should be standard operational mode for Users
- Temperature variation issues for the whole facility and at each beamline must be addressed
- User feedback process could be optimized
- Data preservation policy is needed
- Meeting format lunch to lunch, in general (but obviously not for SAC 19) is preferred
- Phase III evaluation criteria have been proposed and refined