Finalised "ESS nMX STAP End of Meeting Close out report"

Delivered to ESS by the nMX STAP Chaiman October 20th 2014;

3rd Meeting; held ESS Lund September 10-11th 2014

The presented talks are on the ESS indico web page:-

(https://indico.esss.lu.se/indico/conferenceDisplay.py?confId=216).

nMX STAP Members:-

Prof Manuel Angst (FZ Julich, Germany);

Dr Matthew Blakeley (ILL, France);

Prof John R Helliwell (University of Manchester, UK), Chair;

Dr Paul Langan (ORNL, USA);

Dr Derek Logan (Lund University, Sweden);

Dr Sean McSweeney (NSLS, USA);

Prof Nobuo Niimura (Ibaraki University, Japan).

STAP Members' attendance included one (Paul Langan) via conference call and another (Matthew Blakeley) via a skype video link up on the 2nd day; there were no technical issues of communication for the skyoe video link up but the conference call was not so effective (states PL).

Headlines

The extra factor of three calculated flux at the nMX sample from a 'flattened view of the moderator' is most welcome; calculated fluxes of course have to be handled with care.

Great progress has been achieved on the detector question in our opinion, through the involvement of CERN (Dorothea Pfeiffer et al) favouring the 'GEM microstrip technology' and ruling out the very expensive Anger camera as a backup. Thus successive versions of GEM detectors could be installed at nMX, which would gradually improve their absorption efficiency for a consistent spatial resolution (0.2 mm FWHM) with minimal disruption to the user programme.

These two performances, along with the flexible detector placement up to 1m from the crystal sample, would place the ESS nMX with the potential to realise high resolution (~2 Å) studies of biological crystal primitive unit cells of 200 Å up to 300

Å. Thus the ESS nMX instrument is sought as soon as possible in the ESS's development as it is urgently needed.

**** Marvellous progress in a short time on the protein support labs provision (Zoë Fisher).***

****This 3rd STAP is the one immediately following all our inputs to the ESS SAC and thereby on to the 'Steering' Committee in 2013; we have carefully followed their decision requiring us to 'integrate magnetic diffraction into the ESS nMX instrument planning provided it does not compromise nMX'.***

Detailed observations from the STAP now follow:-

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- nMX neutron guide system and choppers look very good, flexible and with low risk;
- MX ancillary labs: there has been great progress in a very short time;
- MX science and engineering staffing looks good - competent personnel, a good team;
- We note relatively simple sample support requirements for the magnetic work;
- We noted the insight from ESS that 10 M€ Anger cameras are not a viable backup plan – being too expensive, and a dead end, was incisive and valuable; we support this self-assessment by ESS;
- The detector group emphasis on the GEM microstrip technology and involvement of CERN detector group looks very healthy. We accept that at ESS nMX instrument start up this technology will likely have poor absorption efficiency but note that nevertheless it will have good spatial resolution (0.2 mm), and it seems that replacing these with better, i.e. more efficient, detectors at a later stage would require minimal down time, which is important.

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- ESS really needs someone to look after the magnetism aspect, namely practical skills, instrument development and assume the local contact role. Such a person could also optimally have experience running a central facility instrument and thus train the others. This person could be shared with or eventually move to another instrument.
- We note the challenge of managing ‘in-kind contributions’;
- End-station software (control and data processing) - control software should definitely be included in the scope, not least for safe operation. Data processing should be achieved during the experiment for all types of experiment and not left to after users depart ESS. The demands being put on DMSC by ESS, with these particular points in mind, are not transparently clear to the STAP. The prime importance of software to data analysis in nMX can for example be illustrated with the headline given in Nature Structural Biology to the first publication in the modern era of nMX and from which we quote:-

> Neutron Laue diffractometry with an imaging plate provides an effective data collection regime for neutron protein crystallography
>
> Nobuo Niimura[1,5], Yoshiaki Minezaki[1], Takamasa Nonaka[2], Jean-Charles Castagna[3], Florent Cipriani[3], Peter Høghøj[4] , Mogens S. Lehmann[4] and Clive Wilkinson[3]
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> **Neutron quasi-Laue diffraction data (2 Å resolution) from tetragonal hen egg-white lysozyme were collected in ten days with neutron imaging plates. The data processing Laue software, LAUEGEN, developed for X-ray Laue diffractometry, was adapted for neutron diffractometry with a cylindrical detector. The data analysis software, X-PLOR, was modified and used for the refinement of hydrogen atoms, and the positions of 960 hydrogen atoms in the protein and 157 bound water molecules, were determined. Several examples are given of the methods used to identify hydrogen atoms and water molecules.**

Nature Structural Biology 1997, 4, 909-914.

End-station software is also a critical aspect for the envisaged materials science applications. For the data processing, clear differences in materials science diffraction data compared to nMX diffraction data need to be taken into account. In particular, materials science experiments will typically yield far fewer reflections than a typical nMX experiment. Indexing of reflections is not based on one large cell, but rather on a small cell plus magnetic or superstructure reflections indexed in terms of a propagation vector and/or several small cells related by twin operations. To provide meaningful access for materials science experimenters, these different needs have to be taken into account in developing beamline end-station software. Alternatively, a second, separate software suite tailored to materials science needs could be developed. In such a case there may even be a very large overlap with software needed for the later-built magnetic diffraction beamline. However, if experimenters with materials science problems are to have access to the earlier built nMX beamline from day 1, it must be ensured that the software is ready when the nMX beamline starts commissioning.

- A formal Memorandum of Understanding with D-lab in Grenoble (http://www.ill.eu/sites/deuteration/) would be a great advantage scientifically, technically ie as a world ranked facility but also politically;
- We are pleased to see a healthy development that the deuteration at ESS will be done in collaboration with LP3, Lund University Protein Production Platform.

- We wonder if we need to have a longer crystal-to-detector distance than 1.0 m, e.g 1.5 m for resolving closely spaced magnetic satellite reflections or resolve Bragg reflections split due to twinning of a superstructure? This is not needed for the vast majority of materials science experiments but would be highly beneficial in some cases (perhaps also in some nMX experiments.).
- We wonder if the STAP should be extended to include one more magnetism representative?
- With the recent approval of ESS for construction, and foundation stone laying completed, the STAP believes that a detailed commissioning plan for nMX including magnetic diffraction is timely.
- Very experienced suppliers, e.g. with multiple installations in facility and user instrument environments should be considered for the end station robotics – we believe that it would be a high risk to focus on just one for the expediency of an 'in kind contribution'.
- A particularly strong case for sample changer robotics would be needed given that remote access will only be possible several years after start up;
- We would like to see a backup plan if the robot arms for holding the detector are delayed or otherwise might fail; we indicate this, along with the detector, as the major experimental station challenge for ESS nMX. Thus we commend that a more detailed examination of the possibilities for the robot arms be investigated fairly soon.

Comments on ESS nMX STAP meeting planning:-
The STAP date of next meeting should be set well in advance;
The STAP meeting frequency would benefit from being at least yearly, perhaps even every 9 months;
Presentation slides and paperwork for the meeting should be provided at least two weeks in advance of the meeting;
A template for the close-out report preferred by the facility should be provided beforehand. This would allow writing assignments to be agreed by the Chair and STAP members before the meeting;
'Cross membership with a magnetism STAP' might be most simply facilitated via a video link with the magnetism STAP Chair at some point during the nMX STAP meeting.

The nMX STAP notes the upcoming TG2 evaluation in December 2014. In anticipation of this ESS provided their self-assessment answers to a set of questions, reproduced below, in consultations both by email and face-to-face with the Chairman at ICCBM15 in Hamburg ie after the STAP meeting. The nMX STAP endorses these answers below as certainly acceptable at this stage of the overall ESS development.

TG 2 Science and Operational Questions

- **Does the scope description match the scientific requirements?**

  We at ESS are confident that for the hardware components the scientific requirements for macromolecular crystallography will be met. The approach to accommodating the materials science case and the associated requirements need to be further clarified including simulations in addition to those presented in the instrument proposal. The software (both control and data processing) that is crucial for the instrument to function is formally not part of the NMX work package scope, but is provided by the ESS Data Management and Software Center. Nevertheless the software components must be described in sufficient detail to assess whether the scientific requirements can be met for both macromolecular crystallography and materials science.

- **Will the instrument meet its stated performance parameters?**

  To the level of confidence that is reasonably achievable at this time we think the expected performance (300 Å unit cell, 0.1-0.01 mm^3 crystal volume, 1 day data collection time) is realistic, especially with the flux gain from the new flat moderator concept. *[ESS nMX STAP comment: We note that these performances will obviously not be realised in each aspect simultaneously.]*

- **Will the instrument meet the needs of its science case?**

  We at ESS are confident that the needs of the macromolecular crystallography science case will be met (see above). The needs for the materials science case must be documented in more detail.

- **Does the layout of the instrument appear to support the operation and use of the instrument?**

  We at ESS feel this is the case. The maintainability is high as all moving parts are out of line-of-sight from the moderator and hence accessible at any time. The control hutch and sample preparation area are large and in close proximity to the experimental cave.

- **Does this instrument meet the users' needs for infrastructure, sample handling, sample manipulation, etc. ?**

  We at ESS are confident that this is the case (see also above). The ESS Scientific Activities Division is responsible for the deuteration and crystal growth facilities, which we feel will be sufficient.

- **Can it be operated safely?**

  We at ESS are confident the instrument can be operated safely. The early loss of line-of-sight along with the doubly redundant shutter system allow for radiation safety. Experimental cave interlocks and hazard detection systems ensure conventional safety for user operations.

- **Do the proposed sample environments and user support facilities meet the needs of the users and match the science case for the instrument?**

With the flexibility at the sample position we are sure the needs can be met with the sample environment equipment available from the ESS sample environment pool.

- **Does the draft commissioning plan sufficiently evaluate the instrument and prove that the instrument works as proposed?**

We at ESS think the plan is sufficiently mature considering the early stage of the ESS project overall, apart from the optics hot commissioning plan that is being developed.

TG 2 Engineering and Project Questions

- **Is the proposal feasible to build?**

We at ESS are confident that the design is feasible to build. The biggest risks are the detectors and the robotic detector positioning system, but risk mitigations exist (see below).

- **Has the team identified all of the appropriate interfaces?**

We at ESS think the interfaces have been identified, but their definition has to be further refined.

- **Has the team implemented the ESS engineering and technical standards where adequate and is ready to follow ESS processes?**

To the extent that such standards and processes exist they have been implemented.

- **Are the cost and duration estimates reasonable?**

These estimates are not yet mature and require work from the instrument team.

[ESS nMX STAP commends that this instrument could be ready in 2019, provided ESS allows that to happen.]

- **Has the team planned appropriately for the risks, both technical and otherwise?**

The risk planning is not yet adequately documented and requires work from the instrument team. The most important risks are associated with the detectors and the robotic detector positioning system and the mitigation strategies need to be documented better.