

ESS Diffraction STAP Report from 24 October 2023 Meeting

STAP had a hybrid meeting with ESS staff and instrument teams present at ESS. STAP members participating were P. Attfield (chair) and M. Angst at ESS; R. Neder, K. Page, H. Playford, G. Rousse, M. Sahlberg and R. Sibille online.

Romain Sibille (PSI) was welcomed as a new member of STAP.

STAP thanks all ESS staff and the instrument teams for their continuing hard work and for the high quality of reports and presentations as below. Recommendations in the report are indicated R and are also listed separately at the end of the report.

Lab Tour

During the morning of 24 October, STAP members in Lund visited the detector testing facility at Utgart (host: Irina Stefanescu) and received presentations on equipment and plans for high magnetic fields (Alex Holmes) and high pressure (Damian Paliwoda).

- Irina and the team are congratulated on a successful detector testing programme. They are keeping up with demand and expect to be busy over the coming years. ESS should ensure sufficient support and suitable working conditions are provided at Utgart. R
- The 8 T magnet being manufactured by LLB is expected at ESS in Q3 2024.
- ESS is part of a European neutron facilities consortium proposal, currently under preparation, to build two magnets that can travel between facilities; a 20 T continuous field magnet, and a pulsed magnet with maximum field 40 T (lasting approx. 50 ms, pulsed every 5 min). These could be used on DREAM and MAGIC (and perhaps HEIMDAL). STAP strongly supports this proposal and notes that the pulsed magnet could be used at the proposed DREAM second sample position, taking occasional neutron pulses to match the duty cycle of the magnet, while standard experiments could run simultaneously at the first sample position with little loss of flux. This would provide a world-leading high-field neutron diffraction instrument for modest upgrade cost. R
- A range of high pressure inserts will be available for hot commissioning (HC) experiments. It will be important to have several people at ESS trained in use of Paris-Edinburgh cells, as these offer the highest pressures (up to 20 GPa) feasible for First Science (FS) and Start of User Programme (SoUP) experiments on DREAM and other instruments. R

Main STAP meeting

STAP received an update on recent ESS developments and presentations from the DREAM, MAGIC and HEIMDAL project teams. DREAM FS was also discussed.

ESS management session and general items

- STAP notes that excellent progress is being made on the ESS project without any significant further slippage of the timetable.
- The need to move DMSC from the present location to the DTU campus is unfortunate. It will be important to maintain staff morale and manage any departures to avoid negative impacts on the start of the ESS neutron science programme. R
- STAP welcomes the recent benchmarking exercise by Pascal Deen, and strongly supports the conclusions that it is of utmost importance to achieve full scope on ESS instruments as soon as possible, ideally before HC and SoUP. R

Diffraction instrument suite

DREAM

DREAM is a bispectral powder diffractometer that will tackle chemistry, physics and materials problems. STAP has emphasised high resolution powder neutron diffraction as the main direction for the science programme.

- STAP notes continuing excellent progress across all areas of the instrument build project. The NBOA, BBG, BSS, guides, shielding, and choppers have been successfully installed/tested. A cold neutron polariser (funded by RAC) is to be installed shortly. A minor issue is regrouting of the T0 chopper base.
- Installation is expected by 7/24 but post-TG5 procedure reviews requested by ESS may add delay – ESS should clarify what will be required. R
- Detector modules are currently being manufactured by CDT and delivered to ESS. A few detector elements were found to have increased background levels (the source was traces of U) but the increased background is within limits and is not expected to cause future issues.
- Full detector coverage is strongly supported by STAP as a first priority. A decision is needed very soon so that the additional elements can be ordered promptly giving the full detector complement at HC/SoUP. With full coverage, DREAM performance is expected to increase from ~25% equivalent to WISH/POWGEN at the start of HC to ~100% equivalence at SoUP. R
- STAP notes good progress with the 20 sample cryostat/cryofurnace.
- The 2nd sample cave (upgrade) would be ideal for a high pulsed magnet endstation, enabling data collection to proceed while the first sample station is also used, as noted above. R

MAGIC

MAGIC is a single crystal instrument designed for magnetism and correlated electron materials studies using polarized cold and thermal neutrons.

- STAP noted excellent progress (choppers, guide, detector, cave) across the project. The solid state bender design is now fixed and the order placed. Recent failures of pulse shaping choppers at high rotation speeds will require remediation (as was done for DREAM after a similar failure).
- Xavier Fabreges is to stand down as MAGIC Instrument Scientist, Xavier is warmly thanked by STAP for his outstanding contributions to this project.
- Staff risks to the project timeline are noted by STAP as an Engineer post is to be readvertised and the Instrument Scientist position needs to be refilled. ESS will need to monitor this aspect. R
- Only 75% of the wide angle polarisation analyser is affordable according to a recent costing. This would lead to an unacceptable loss of performance and STAP strongly endorses efforts to find funds for the remaining 25% to complete the full scope of the wide angle polarisation as the highest priority for MAGIC. R

HEIMDAL

HEIMDAL will offer a combination of powder neutron diffraction, small angle neutron scattering (SANS) and neutron imaging to enable complex and evolving systems to be studied over multiple length scales.

- STAP notes excellent progress with construction started and the NBOA installed.
- Appointment of an additional Engineer is welcomed.
- Plans to have in-bunker installation completed before BOT are on track and are strongly supported by STAP.
- The guide contract including thermal and 116m of cold guide is now awarded.
- The detector contract has been awarded to CDT. This currently covers 1.0 sr, an upgrade to 1.3 sr is strongly encouraged by STAP. R
- Cave redesign to use smaller modular 'Lego' blocks is strongly supported by STAP. This will give flexibility for future cave changes to include and later upgrade the SANS tank. R
- A consequence of the above, and also a request by ESS to have access to pillar supports around the sample position, is that the HEIMDAL team are considering a possible move of the sample position from 157 to 158 m. STAP notes that this will require full and careful consideration in consultation with ESS. R

DREAM First Science

- STAP and the instrument team members found the First Science discussion for DREAM to be a useful exercise. Several ideas papers were provided (by the DREAM team and two STAP members; P. Attfield and G. Rousse) and these will be combined into a single document for further discussion at the next STAP meeting. ESS might wish to recommend a similar process for all instruments, to start ~2 years before HC. R

- STAP thanks all contributors and notes general agreement to progress from beamline characteristic studies through standard to ~10 more complex (new science) experiments such as magnetism and battery materials.
- As noted above, DREAM performance is expected to increase from ~25% equivalent to WISH/POWGEN at the start of HC to ~100% equivalence at SoUP. This is sufficient for the above FS assuming ~80-120 days are available for HC.
- Plans for measuring PND, PDF, single crystal and polarised SANS standards at low, medium and high-resolution chopper settings as initial beamline characteristic studies are useful for defining instrument resolution functions, but this is a lot of work and risks loss of focus which should be on high resolution PND to fulfil the science case. R
- Many exciting science ideas are already proposed. Plans to coordinate sample provision and synthesis will be needed, with timings clear to ESS staff and external collaborators.
- ESS should consider some general issues for HC/FS. How much beamtime will be available? Will external 'friendly' users receive travel support, accommodation, etc? Access arrangements for external users (radioprotection, etc)? Agreements on collaboration and publications? R
- STAP proposes to conduct a similar FS exercise for MAGIC at the October 2024 meeting. R

Summary of Diffraction STAP Recommendations (7 and 10 are high priority)

1. Irina and the team at Utgard are congratulated on a successful detector testing programme. ESS should ensure sufficient support and suitable working conditions are provided at Utgard. R
2. ESS is part of a European neutron facilities consortium proposal, currently under preparation, to build two magnets that can travel between facilities. STAP strongly supports this proposal and notes that the pulsed magnet could be used at the proposed DREAM second sample position to provide a world-leading high-field neutron diffraction instrument for modest upgrade cost. R
3. It will be important to have several people at ESS trained in use of Paris-Edinburgh cells for First Science (FS) and Start of User Programme (SoUP) experiments on DREAM and other instruments. R
4. The need to move DMSC from the present location to the DTU campus is unfortunate. It will be important to maintain staff morale and manage any departures to avoid negative impacts on the start of the ESS neutron science programme. R
5. STAP welcomes the recent benchmarking exercise by Pascal Deen, and strongly supports the conclusions that it is of utmost importance to achieve full scope on ESS instruments as soon as possible, ideally before HC and SoUP. R

6. DREAM installation is expected by 7/24 but post-TG5 procedure reviews requested by ESS may add delay – ESS should clarify what will be required. R
7. **Full DREAM detector coverage is strongly supported by STAP as a first priority. A decision is needed very soon so that the additional elements can be ordered promptly so that the full detector complement is available at HC/SoUP. R**
8. The 2nd DREAM sample cave upgrade would be ideal for a high pulsed magnet endstation, enabling data collection to proceed while the first sample station is also used. R
9. Staff risks to the MAGIC project timeline are noted by STAP. ESS will need to monitor this aspect. R
10. **Only 75% of the MAGIC wide angle polarisation analyser is affordable according to a recent costing. STAP strongly endorses efforts to find funds for the remaining 25% to as the highest priority for MAGIC. R**
11. The HEIMDAL detector contract has been awarded to CDT. This currently covers 1.0 sr, an upgrade to 1.3 sr is strongly encouraged by STAP. R
12. HEIMDAL cave redesign to use smaller modular ‘Lego’ blocks is strongly supported by STAP. R
13. The HEIMDAL team are considering a possible move of the sample position from 157 to 158 m. STAP notes that this will require full and careful consideration in consultation with ESS. R
14. STAP and the instrument team members found the First Science discussion for DREAM to be a useful exercise. ESS might wish to recommend a similar process for other instruments, to start ~2 years before HC. R
15. DREAM FS focus which should be on high resolution PND to fulfil the science case. R
16. ESS should consider some general issues for HC/FS. How much beamtime will be available? Will external ‘friendly’ users receive travel support, accommodation, etc? Access arrangements for external users (radioprotection, etc)? Agreements on collaboration and publications? R
17. STAP proposes to conduct a FS exercise for MAGIC at the October 2024 meeting. R