

ESS Diffraction STAP Report from 16-17 April 2024 Meeting

STAP had an online meeting with ESS staff and instrument teams. STAP members participating were M. Angst, P. Attfield (chair), R. Neder, H. Playford, G. Rousse, M. Sahlberg and R. Sibille.

STAP thanks 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.

Common STAP Sessions on 16 April

- STAP notes that excellent progress is being made on the ESS project and good efforts are being made to define and stay within the critical paths in the timetable.
- Quality issues in concrete blocks supplied for the bunker roof and potentially other parts of ESS by a particular manufacturer raise a significant risk of delay to the BoT and other milestone dates, and any such delays should be communicated to the community. R
- The move of DMSC to the DTU campus has been successful but has significantly increased travel times from DMSC to ESS-Lund. It will be important to allow flexible working and perhaps locations of DMSC staff to avoid negative impacts on the ESS start-up and neutron science programme. R
- Documentation required for TG5 needs to be clarified by ESS soon so instrument teams can prepare in good time. R
- Continuing recruitment of Engineers is clearly important to keep the ESS project on track.
- Rebaselining of Tranche 2 and 3 instruments is a worthwhile exercise to provide realistic milestone dates for the latter parts of the ESS project. It will also be important to mitigate cost increases resulting from delays for later instruments. R
- STAP members found the joint presentation and discussion session very useful and recommends that this format is used at future STAP meetings. This will enable dates for future STAP meetings to be circulated at least a year in advance, which will be helpful for STAP members wishing to fix dates for travel. R

Diffraction STAP Sessions on 17 April

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

DREAM

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

- STAP notes continuing excellent progress across all areas of the instrument build project, as also mentioned in many of the Common STAP presentations.
- Mikhail Feyngenson is congratulated on his appointment as the Diffraction & Imaging Division Head. It will be important to recruit a replacement for the DREAM project soon. R
- Continuing installation and testing of beamline components is noted. Regrouting of the T0 chopper base has been done. The cold neutron polariser funded by RAC is being installed.
- Successful testing and installation of the endcap detector modules is noted. Full detector coverage is still strongly supported by STAP as a first priority. R
- Plans for manufacture of a 20 sample cryostat/cryofurnace have fallen through and a new design and tender is being considered. STAP supports continuing efforts to try to realise this equipment, but also recommends planning for use of the 100-1073 K gas blower with robot capillary sample changer plus conventional cryostats to support early DREAM science. R
- The proposed installation of a sprinkler system in the DREAM and other instrument caves is considered highly risky given the potentially ruinous damage that could result from accidental activation. STAP recommends that ESS considers this extremely carefully. R

MAGIC

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

- STAP noted excellent progress across the project.
- A new Engineer is in post and it remains important to recruit an Instrument Scientist to replace Xavier Fabreges. R
- Good progress across beamline components is noted; chopper, guide, detector, cave, monitors, pulse shaping choppers, and the solid state bender. Slight delays to delivery of guide and vacuum housing are not critical.
- Only 75% of the wide angle polarisation analyser is affordable according to recent estimates and STAP continues to strongly endorse efforts to find funds for the remaining 25% as the highest priority for MAGIC. R
- TG5 is now expected in 2026 and it will be important to provide the rebaselined timetable soon. R

- A benchmarking exercise shows that MAGIC will be competitive with comparator instruments (WISH, D7, DNS) from the start. This will enable an exciting First Science programme to be drawn up and STAP proposes to start this in 2025. R

HEIMDAL

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

- STAP notes excellent progress with construction now underway.
- The new Engineer is welcomed and another appointment will be needed soon in view of an impending retirement. R
- Good progress to build the thermal and 116 m of cold guide through active development of the design with the manufacturer is noted.
- This currently planned detector covers 1.0 sr, an upgrade to 1.3 sr is still strongly encouraged by STAP. R
- Quality control and financial issues experienced by the company awarded the contract to build the cave from small modular 'Lego' concrete blocks may require termination of the contract. A new tender, perhaps combining the cave and cabin builds, and choice of supplier may offer the most time- and cost- effective way forward. R
- Rebaselining will be important to provide a realistic timetable for HEIMDAL. It will also be important to mitigate cost increases resulting from the delay to this instrument build. R

DREAM First Science

- A second discussion of First Science for DREAM was a useful exercise and STAP thanks all contributors and notes general agreement to progress from beamline characteristic studies through standard samples to more complex experiments on new materials such as magnetics and battery materials.
- STAP recommends that the focus for DREAM remains on high resolution PND while also testing other capabilities such PDF, single crystal and polarised SANS during commissioning. R
- STAP thanks Céline Durniak for providing a paper on DMSC activities related to DREAM First Science. This demonstrates the pipeline for data processing and analysis by the user through use of the EasyDiffraction interface. STAP recommends that some powder structure refinements against simulated DREAM data are carried out using standard software such as FullProf or GSAS as experienced users are likely to expect such demonstrations. R
- STAP proposes that an outline DREAM First Science paper will be co-written by a member of the instrument team and a member of STAP. Mikhail Feygenson and

Romain Sibille are warmly thanked for volunteering to take on these respective roles. This document will draw on ideas papers provided by the DREAM team and STAP members at the last meeting, and by DMSC as above. A call for any further inputs will be made in September 2024 and the paper will be submitted for the October 2024 STAP and SAC meetings. ESS could consider a similar process for all instruments. R

- It was noted that many exciting new materials for high resolution structural or magnetic PND analysis are produced by the scientific community each year. Several STAP members can offer access to such samples. STAP recommends that specific materials for HC studies are selected at the October 2025 meeting (assuming BoT in July 2025 with HC thereafter in Q4 2025). R
- STAP again notes that it will be important for ESS to 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

Summary of Diffraction STAP Recommendations (7, 11, 15 are high priority)

1. Quality issues in concrete blocks raise a significant risk of delay to the BoT and any such delays should be communicated to the community. R
2. The move of DMSC to the DTU campus has significantly increased travel times from DMSC to ESS-Lund so flexible working and perhaps locating of DMSC staff may be needed. R
3. Documentation required for TG5 needs to be clarified by ESS soon so instrument teams can prepare in good time. R
4. Rebaselining of Tranche 2 and 3 instruments should provide realistic milestone dates and be used to mitigate cost increases for later instruments. R
5. Use the initial joint presentation and discussion session at future STAP meetings with dates for future STAP meetings circulated at least a year in advance. R
6. Recruit a replacement for Mikhail Feygenson for the DREAM project soon. R
- 7. Full DREAM detector coverage is still strongly supported by STAP as a first priority. R**
8. Continue efforts to try to realise a 20 sample DREAM cryostat/cryofurnace, but also plan for use of the 100-1073 K gas blower with robot capillary sample changer plus conventional cryostats to support early science. R
9. The proposed installation of a sprinkler system in the DREAM and other instrument caves is considered highly risky and STAP recommends that ESS considers this extremely carefully. R
10. Recruit a MAGIC Instrument Scientist to replace Xavier Fabreges. R
- 11. STAP continues to strongly endorse efforts to find funds for the remaining 25% of the wide angle polarisation analyser as the highest priority for MAGIC. R**
12. Provide the rebaselined MAGIC timetable soon. R

13. Start MAGIC First Science planning in 2025. R
14. HEIMDAL Engineer appointment will be needed soon in view of an impending retirement. R
- 15. Upgrade of HEIMDAL detector coverage from 1.0 to 1.3 sr is still strongly encouraged by STAP. R**
16. A new tender and choice of supplier may offer the most time- and cost- effective way forward for the HEIMDAL cave (and cabin). R
17. Rebaseline to provide a realistic timetable for HEIMDAL and mitigate resulting cost increases. R
18. STAP recommends that some powder structure refinements against simulated DREAM data are carried out using standard software such as FullProf or GSAS. R
19. STAP proposes that an outline DREAM First Science paper will be co-written by a member of the instrument team and a member of STAP. ESS could consider a similar process for all instruments. R
20. STAP recommends that specific materials for HC studies are selected at the October 2025 meeting (assuming current ESS timetable). R
21. STAP again notes that it will be important for ESS to 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