ESS Diffraction STAP Report from 22-23 October 2024 Meeting

STAP had a meeting with ESS staff and instrument teams at ESS. STAP members participating were P. Attfield (chair) and M. Angst, R. Neder, H. Playford, and R. Sibille at ESS; and G. Rousse online. M. Sahlberg was absent on family leave.

Reinhard Neder is standing down and he was warming thanked for his contributions to STAP over many years.

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 and main points in the report are indicated in **bold** and are also listed separately at the end of the report.

Lab Tour

During the morning of 22 October, STAP members in Lund visited ESS. Impressive progress on the instrument builds, e.g. DREAM detectors and MAGIC cave, were noted.

Main STAP meeting

STAP received an update on recent ESS developments and presentations from the DREAM, MAGIC and HEIMDAL project teams, also on ESS electrochemistry capabilities, high pressure planning, and data processing. DREAM FS was also discussed.

General items

- STAP notes that excellent progress is being made on the ESS project with a clearly defined timetable leading up to end of construction in 2027 and the start of the user programme in 2028.
- **An Expression of Interest (EoI) process for instruments 16-22 to start in 1/2025 is noted. STAP will be happy to review outline EoI cases. STAP emphasises that a dedicated high pressure diffraction beamline remains a priority to fill an important scientific capability gap in the diffraction suite.**
- **STAP endorses rescoping plans presented by the Diffraction and Imaging Group Director, with proposed detector coverage of DREAM, HEIMDAL, MAGIC as first priorities. Scheduling of detector module production with CDT needs careful consideration. STAP looks forward to more details and decisions on the rescoping plan at the Spring STAP meeting in 2025.**
- **STAP noted that arrangements for argon/carbon dioxide gas mixing and supply to CDT detectors and monitors requires consideration (more details under DREAM). There is a potentially widespread and long term risk to ESS detectors that requires mitigation.**

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 of the instrument project with good progress on Utilities, Choppers, Cave, and Detector installations. A slight delay in arrival of mantle detector elements is not limiting.
- STAP congratulated Florence Porcher who has been appointed as DREAM lead scientist. Ongoing appointments of a commissioning scientist position (with Uppsala Univ.) and an initial operating engineer (IOE) were also noted positively.
- Good progress on data reduction, export, and analysis with standard programs for powders was noted. It may be useful to anticipate workflows for single crystals on DREAM, although the focus remains on powder diffraction.
- **STAP learnt of a requirement for flowing Ar/CO_2 gas (without O_2) to be passed continuously through CDT detectors and monitors during operation. This raises some important questions for Diffraction and probably other ESS Groups for the engineering of systems for gas mixing and flow through many modules. STAP queries whether the required Ar/CO_2 gas flow through CDT detectors raises long-term issues, e.g. do variations in gas proportions/flow rate/pressure affect detector performance, corrosion, or fouling through carbonate formation? Using premixed Ar/CO_2 gas cylinders is a useful interim solution for detector testing while the above issues are addressed. [STAP repeats its previous view that some long term testing of detectors in a pulsed neutron beam would be useful.]**
- The design and build of a DREAM cryostat/cryofurnace with a 20 sample changer is still unclear. STAP notes that use of a gas blower (100-1073 K) and conventional cryostats provide a good mitigation plan during the early science period.
- **Full detector coverage (from the present 41% to 100% of original coverage) is still strongly supported by STAP for rescoping as a first priority.**

MAGIC

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

- STAP notes excellent progress across all areas of the instrument project. The cave has been installed very smoothly. Good chopper, guide, detector, cave, monitors, PSC, bender, analyzer progress is noted. A vacuum housing delay could be on the critical path for in-bunker installation.
- STAP welcomed Denis Vasiukov – MAGIC instrument scientist (from 12/24), and Moritz Braun – newly appointed Engineer.

- Rebaselined timing is noted – TG5 will be in 2/27.
- **MAGIC First Science planning by STAP will start at the April 2025 meeting, in anticipation of MAGIC First Science in Q1 2027. Manuel Angst (STAP) and Denis Vasiukov (MAGIC) have kindly agreed to coordinate the FS paper.**
- **STAP supports the proposed rescoped detector coverage.**
- STAP notes that a simple spectroscopy option could be a worthwhile future upgrade to MAGIC.

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 across installation/manufacture/planning of the NBOA, choppers, thermal and cold guides, detectors, and shutters.
- STAP welcomed the new lead engineer Siamak Kianzad, and notes that another engineering appointment is likely to be needed soon.
- The new TG5 target of Q3 2027 is ambitious but STAP feels it is realistic with provision of sufficient resources.
- **Upgrade of detector coverage from 1.0 to 2.0 sr (and later to 3.0 sr) is strongly supported by STAP. STAP discussed the idea of using a 1.0 sr movable detector but this is not recommended for the long term as it limits much of the science case for which variable time, *T*, etc experiments are important. A 1.0 sr movable detector could at best be a temporary solution during initial HEIMDAL experiments.**
- A SANS rescope, adding the final 25% of the cold guide with flux gain from redesign is also supported by STAP.
- STAP notes that communications with the cave manufacturer will require careful attention and monitoring.
- **STAP proposes to start HEIMDAL FS paper preparation at the 10/25 meeting.**

DREAM First Science

- STAP thanked Romain Sibille and Florence Porcher for writing the presented Outline Paper, and all contributors.
- **A plan is now in place to progress from beamline characterisation studies through standard to more complex (new science) experiments such as on magnetism, MOFs and battery materials (including in situ setups – where testing pre-existing PND cells may be useful). Many exciting science ideas and samples are noted.**
- **Detailed responsibilities for samples to be provided by ESS and STAP people were assigned.**

- STAP reiterated that FS should keep a focus on high resolution PND (including analysis with standard software – FullProf, GSAS, etc) while also testing PDF, single crystal and polarised SANS during commissioning.
- **STAP notes ESS-RCO issues under consideration: How will HC time be allocated? Can outside 'friendly' users come? Travel/accommodation arrangements and reimbursement? Collaboration/publication policy?**

Summary of Diffraction STAP Main points and Recommendations

General

- **An Expression of Interest (EoI) process for instruments 16-22 to start in 1/2025 is noted. STAP will be happy to review outline EoI cases. STAP emphasises that a dedicated high pressure diffraction beamline remains a priority to fill an important scientific capability gap in the diffraction suite.**
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