ESS Diffraction STAP Report from 19-21 October 2020 Meeting

Members of the ESS Diffraction STAP joined the ESS management Q&A session on 19 October and the joint DMSC-STAP session on 20 October.

The whole STAP met by videoconference on 21 October with ESS staff and instrument teams. All STAP members participated; M. Angst, P. Attfield (chair), T. Fennell, K. Page, R. Neder, G. Rousse, O. Zaharko.

STAP received presentations on recent ESS developments, from the DREAM, MAGIC, and HEIMDAL project teams, and on the test of the POWTEX Jalousie-type detector at SNS. STAP is grateful to all ESS staff and the instrument teams for their continuing hard work during current covid-restricted times, and for the high quality of reports to this meeting.

ESS management Q&A session

- STAP noted that some delays to the ESS construction and start-up due to coronavirus issues have been incurred. It will be important to update key dates like SOUP to the user community as start of ESS neutron science becomes closer. This could be done after the planned rebaselining exercise in the first half of 2021.
- Initial wide consultations on the First Science programme are sensible. However, it will then be important to narrow down the list of early experiments to provide a focussed programme. It should be clear who has leadership for each instrument.

DMSC-STAP session

- Further progress on the ESS easyDiffraction software using the standard CrysPy and CrysFML libraries is noted. Smooth transfer of data from ESS data reduction programs to standard external packages like Fullprof, Jana, GSAS-II will be important to First Science on DREAM, and this should be checked in good time. STAP encourages close consultation between DMSC and the DREAM and HEIMDAL teams with respect to 2D-Rietveld refinement.
- STAP supports the use of SCIPP to replace Mantid.
- Remote and scripting options are likely to be important parts of instrument control software. STAP has noted early needs for Sample Environments in DREAM and MAGIC reports.

Diffraction instrument suite

Detectors

- Following previous STAP concerns about experimental testing of the Jalousie type detectors under realistic neutronic conditions (i.e. on intense pulsed sources over appreciable periods of time), a report on testing of the POWTEX mantle detector on the POWGEN@SNS beamline in 2017 was presented.
- STAP noted that useful testing had taken place over a period of around 1 week, despite damage to the detector during transit.
- Diffraction data from a standard diamond powder appears visually to be of good quality. However, it will be important to establish quantitative aspects of the data through normalisation of the spectra including any data stitching, and Rietveld fitting of diffraction intensities over a few orders of magnitude.

DREAM

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

Specific comments from the present meeting;

- STAP notes continuing excellent progress across the instrument build project with no critical risks apparent. DREAM remains on schedule to be one of the 'first 3' ESS instruments for users.
- Investigation of whether collimators may be needed, e.g. to reduce background from the sample environment when measuring small samples, should be undertaken as recommended in the previous STAP report.
- The planned 20-sample cryofurnace to cover the range 4-800 K is still strongly supported by STAP. However, if this build proves too challenging then fallback options such as by using gas blowers may be needed.
- Provision of a second sample station and a fuller detector coverage remain the highest priority upgrades in STAP's opinion. The cost-effectiveness of including the second sample station during the initial build should be remembered in the coming weeks as tenders for the DREAM Cave are considered. The presented thermal polarisation option is also potentially worthwhile as a future upgrade. Cold polarised neutrons are already covered in the RAC-funded upgrade.

- The DREAM team in encouraged to keep in close consultation with ESS management and the ODIN team regarding the maximum floor loading capabilities of the experimental caves.
- P. Attfield and G. Rousse will help to develop the Hot Commissioning and First Science experiments. The following sequence is suggested;
    - Initial experiments without SE – room temperature analysis of simple standard materials, some functional e.g. energy or electronic materials, simple (room temperature) magnetic structures, and analysis of a more complex unknown structure e.g. a MOF.
    - 1D and 2D fits during the above to explore and optimise data fitting strategies.
    - Variable T SE experiments; low T for magnetism, high T for phase transitions and some simple chemistry experiments such as decomposition or oxidation.
    - Other SE experiments; high magnetic field or pressure, and *in situ* battery, catalysis, or reaction cell experiments.

MAGIC

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

STAP comments on the information provided at the present meeting;

- STAP notes excellent progress across almost all areas of the project, although the wide-angle polarisation analyser is a concern as discussed below.
- Some local issues at LLB in the Cave tender process need to be resolved as a priority to avoid delays to the project path.
- The change in design to the solid state bender is noted and supported. The available field of 1 – 2 kG is likely to be sufficient.
- STAP appreciated the separate report on the wide-angle polarisation analyser. Provision of analyser coverage over 120 degrees is challenging but important to the MAGIC science case. The report's conclusion that a solid state device appears the best solution is accepted, but sensitivity to misalignment of the elements leading to loss of performance is identified as a critical issue. If this cannot be ameliorated then alternative solutions like a bender may be needed. A long build time of 3 – 6 years is envisaged so it is desirable to add segments of the analyser to the instrument in stages, as soon as they are ready, to provide some polarisation options to users. Provision of this analyser is identified as a critical path issue to the science programme of MAGIC.

- First Science experiments on MAGIC are likely to require very low temperatures (< 2 K) and high magnetic fields. M. Angst, T. Fennell, and O. Zaharko have kindly agreed to help develop the Hot Commissioning and First Science programme.

HEIMDAL

HEIMDAL will offer a combination of powder neutron diffraction (PND) and small angle neutron scattering (SANS) and eventually neutron imaging to enable complex and changing systems to be studied over multiple length scales. Separate guides and detectors for the cold and thermal neutron spectra are planned.

STAP comments from the present meeting;

- STAP notes continuing good progress although with a slight delay as Swiss Government approval for funding of the PSI contribution has been delayed until early 2021.
- Progress on the planned Change of Scope request is needed to give clarity over the instrument build and First Science programme. STAP encourages the HEIMDAL team and ESS to work together on this. A clear timetable is needed. STAP notes the ambition for this issue to be decided by the April 2021 STAP and SAC meetings, but this deadline may prove overambitious.
- STAP continues to support the original science case to which simultaneous PND and SANS measurements are fundamental. Inclusion of the cold guide in the initial build will be prerequisite to a polarisation upgrade.
- The project of a PhD student at Aarhus University to develop 2D Rietveld fitting methods is warmly welcomed by STAP. This provides a good way for the HEIMDAL team to be involved in early Diffraction science at ESS.