ESS Diffraction STAP Report from 24 April 2020 Meeting

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

STAP received presentations on recent ESS developments and from the DREAM, MAGIC, and HEIMDAL project teams in advance and circulated initial questions. Feedback on these questions formed the basis of discussion during the videoconference. STAP is grateful to all ESS staff and the instrument teams for their continuing hard work including the high quality of reports to this meeting.

ESS Reports

ESS presentation

- STAP congratulated and welcomed Andrew Jackson as Instrument Scientists Group Leader.
- Re-organisation, common projects, and continuing construction progress were noted positively. It will be important to encourage instrument scientists to pursue their own scientific programmes as well as beamline and community developments.
- STAP notes that delays to the ESS construction and start-up due to coronavirus issues are likely, and the next meeting in October will be a sensible time to assess their extent. None of the Diffraction suite instruments expect significant delays over what is likely to occur across the whole ESS project.
- As a general First Science milestone, to be confirmed by 9 months before BOT, STAP suggests the refinement of a crystal structure of an interesting new functional material using powder diffraction data collected on DREAM.
- STAP looks forward to the combined autumn STAP and SAC meeting. STAP plans to cover all business items in a day (Wednesday 21st October) with an optional site tour (if available) and dinner beforehand on Tuesday 20th.

Polarisation

- STAP welcomed Hal Lee as leader of this project to ESS.
- STAP agrees with the underlying premise that is it more cost-efficient to coordinate polarisation upgrades and include these within instrument builds than to retrofit them later. However, the likely funding for polarisation upgrades from the Initial Operations budget inevitably reduces funding for other upgrades and cross-instrument activities e.g. sample environments. STAP will welcome an outline budget of the polarisation project for discussion at our next meeting.

- MAGIC is already designed as a fully polarised instrument. STAP has previously prioritised other upgrade options for DREAM and HEIMDAL over polarisation; notably the second sample station and increased detector coverage for DREAM, and the cold guide for HEIMDAL. The impression that these important items have been deprioritised in favour of less-requested polarisation options would be unlikely to be well received by the user community.
- STAP notes that additional external funding may be accessible for early polarisation upgrades, such as that recently obtained for DREAM via the Swedish-German Röntgen-Ångström Cluster (RÅC) research collaboration.

DMSC

- DMSC progress such as focus on DREAM and ODIN data treatment is noted positively.
- Interfacing of easyDiffraction to standard libraries like CrysPy and CrysFML are further positive developments. Interfacing ESS software to Fullprof and other standard packages will be essential to users. These should be beta tested by experienced users with simulated data before ESS HC.
- Interfacing of data acquisition and instrument control software will be highly important and there is a potential bottleneck of many initial instruments with diverse detector and control hardware all wishing to do this at the same time. ESS management should ensure that should ensure that DMSC and the various instrument teams are working closely together to prepare in advance and minimise delays.

SAD

- STAP notes positive developments in many important areas such as the Scientific Coordination and User Office, Laboratories, and Sample Environments.
- Excellent progress on the 8T magnet (for MAGIC in particular) is noted.
- A 20-sample cryofurnace for DREAM is ambitious but a similar SE is planned for SNS and it may be possible for the manufacturer to tender to ESS.

Diffraction instrument suite

Detectors

- Simulations of detector performance are making excellent progress.
- STAP is concerned that experimental testing of the Jalousie type detectors to be used on all three instruments under realistic neutronic conditions (i.e. on intense pulsed sources over appreciable periods of time) has not progressed since this issue was raised at the last meeting. This issue was not identified as being on the critical path earlier because modules were supposed to be tested on POWTEX@FRM-II but this has not happened. Coronavirus is now adding further delays to other testing options, but in our view it is imperative to arrange tests of Jalousie detector modules on spallation instruments soon, e.g. at ISIS or SNS.
- Experimental verification of detector performance is becoming a critical risk for the entire Diffraction suite, in STAP's view, and it is not clear what steps are being taken to mitigate this risk.

DREAM

DREAM is a versatile powder diffractometer that can tackle many chemistry, physics and materials problems. STAP has previously endorsed the science case with emphasis on high resolution powder neutron diffraction.

Specific comments from the present meeting;

- STAP congratulated Mikhail Ferguson on his appointment to an ESS staff position from mid-2021. His move from the current DREAM build team will be phased so that no delays to the instrument construction are expected.
- STAP notes that the team have made continuing excellent progress and no significant delays over what is likely to occur across the whole ESS project are anticipated. DREAM remains on schedule to be a 'first 3' instrument for SOUP.
- TG3 is planned for 12/2020. Many packages are to be checked that month so some delays into early 2021 are possible, but these are not expected to delay the overall build.
- The plan to acquire a 20-sample cryofurnace to cover the range 4-800 K is strongly supported by STAP. A design may be available from SNS as noted above. Reducing scope to cover only low temperatures may be necessary if funds are limited, and use of standard cryostats and furnaces is a valid fallback position.
- Provision of a collimator may be important even for early science, e.g. to reduce background from the sample environment when measuring small samples, although this is currently outwith the supported instrument scope. This is another important early upgrade for DREAM.

- A strong programme of detector simulations is underway, but real testing on intense pulsed neutron beams remains a concern as noted above, especially as the DRAM detector is to be ordered soon, in Q3-2020.
- The scenario of chopper disks having to be installed after the DREAM bunker closing date should be avoided if at all possible, and this should kept under review as the timetable evolves.
- The team are congratulated on their success in obtaining funding for construction of a SANS detector and polarizer via the Swedish-German research collaboration Röntgen-Ångström Cluster (RÅC). This will add further valuable scope to the instrument, but the focus should remain on high resolution powder diffraction as the early science priority for DREAM.

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 all areas of the project including agreement on VAT arrangements with PSI, and coordination of xyz polarisation plans across the 3 groups.

- No significant delays over what is likely to occur across the whole ESS project are anticipated. HC is on track for early 2023.

- Detector plans are on schedule, subject to above caveats.

- Plans to modify the guide design, replacing the fully elliptical model with two half-ellipses to reduce costs, are supported by STAP. The planned increase of bender field is unaffected. Manufacture of the guide in 4 separate lots is feasible as their precise interconnections are not critical.

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 with all TAs now approved. HEIMDAL is further upstream than other Diffraction suite instruments so no further delays over those likely across the whole ESS project are expected.
- STAP continues to encourage the HEIMDAL team and ESS to come up with agreed costs for major components to inform the planned Change of Scope request. A clear timetable is needed for this process. STAP would like to have the case substantially in place for the next meeting in October so submission can take place soon afterwards. A clear decision and plans for the way forward based on whether the request is accepted or denied should be in place by April 2021.
- STAP reiterates the original science case and notes that inclusion of the cold guide in the initial build will be essential to take advantage of any proposed polarisation upgrade.
- ESS should establish a clear timetable for appointment of a staff scientist to run HEIMDAL, keeping the build team members informed.