ESS Diffraction STAP Report from 22-23 June 2016 meeting

The ESS Diffraction STAP (M. Angst, P. Attfield (chair), T. Fennell, S. Hull, R. Neder, K. Page, G. Rousse, O. Zaharko) met at the Grand Hotel, Lund during 22 and 23 June 2016, and visited the ESS construction site during the morning of 23 June.

STAP received presentations from the DREAM, MAGIC, and HEIMDAL project teams, and was asked to comment upon the following aspects;

- which parts of the science case for diffraction should be covered by this instrument?
- to what extent does the instrument design match that science case?
- are the proposed technical solutions sound?
- is the project plan mature and realistic?
- are the plans for sample environment for day 1 and early operations appropriate?
- what are the scientific priorities for realising the instrument scope?
- which capabilities must be available on day 1 (minimum acceptable scope)?
- rank the capabilities which could be brought in through upgrades

STAP’s reviews of the instruments below are followed by general comments from several themes that emerged in discussion and are reported here for ESS to consider.

DREAM

Science case

DREAM is a versatile powder diffractometer that can efficiently tackle many scientific cases from fundamental to applied science in physics and chemistry. DREAM will be ideal to study magnetic compounds and magnetic systems with emphasis on compounds presenting small magnetic moments, orbital and charge ordering phenomena. It also aims at addressing compounds presenting light elements (Li, Na, H…) in a crystallographic way with the study of new compounds (high resolution powder diffraction), and further to examine their behaviour *in situ* or *operando*. The latter case includes time-resolved/parametric studies of batteries during charge and discharge, hydrogen storage compounds, MOFs, etc. DREAM will also make it possible to perform neutron diffraction experiments on very small samples (e.g. in pressure cells). Nano-objects and core-shell compounds will be addressed thanks to the cold and thermal neutrons available in the incident neutron beam, and single crystal (TOF Laue) diffraction will complement the scientific capabilities. DREAM will address scientific cases ranging from superconductors and multiferroic systems to energy storage systems, to cite only a few.

Technical Design

DREAM's mission to be a Day 1 general purpose powder diffractometer for a broad user community requires high intensity, high resolution, high signal to background ratio performance and sample environment (SE) allowing rapid change of samples. Technical design of the instrument is focused on these demands and is at a mature stage.

The instrument has been optimized for the new ESS butterfly moderator, a Si-wafer stack replaces the solid-state bender as a better option to extract the bispectral beam. The choppers and neutron optics, as well as shielding and the beamstop, and the sample station are defined by the instrument team. They need to be verified by simulations and calculations by ESS.

Much thought has been given to the detector design, and preference has been given to the “Jalousie” type (cathode layers covered with 1 µm ^{10}B) for the 90-deg, backscattering and forward scattering detectors. The instrument team has a concern about the compromises to be made due to budgetary issues on the detector volume (e.g. 12- or 10- layers), the angular coverage (1-6 sr) and also on the priority of the positioning of the detectors. Ideas for a second sample station (for alignment, preparation, testing the samples to be measured at the main station, and running a possible high pressure programme), single crystal and even a polarization option are sketched out.

STAP comments

STAP feels that the DREAM science case remains relevant and worthwhile. The focus should be on delivering a high resolution powder diffractometer on Day 1 that offers world-beating resolution down to $\Delta d/d = 2.8 \times 10^{-4}$ at long wavelengths as part of wide-Q data. Software developments for 2D Rietveld analysis are underway with a proof-of-concept publication already available, and STAP felt that such supportive external contributions from the community will be a useful path towards productivity from Day 1. Other useful DREAM capabilities are to provide total scattering data up to Q = 20-25 $Å^{-1}$ for PDF use, and some single crystal capabilities to complement MAGIC once a large detector coverage is available. SANS data collection is of lower priority as other instruments are available, and polarization is also of less importance given the availability of MAGIC.

The project plan is mature and options have been evaluated realistically including a move to the S3 beam port. The basic instrument design will deliver the above high resolution powder diffraction capability. STAP feels that construction of a high quality primary flightpath including a T0 chopper is important. STAP recommends that high quality (e.g. 12-layer, subject to technical decisions) B-10 detectors are used to ensure high counting efficiency that will aid fast experiments. A large detector coverage is essential to the long term success of DREAM. Provision of 1 sr on Day 1 is the absolute minimum to provide a working instrument, and a coverage significantly greater than 1 sr will be needed if DREAM is to contribute to the "early success" strategy of the ESS. If the full coverage cannot be realized within the initial construction budget, plans should be made for a speedy upgrade to the 4-6 sr coverage that will be needed to cope with the expected user demand. We suggest that backscattering and 90 deg detectors are prioritised over forward scattering banks. Reduction of air-scatter is also desirable, especially when dealing with small samples or rapid counting. The SE request is appropriate. Sample changers for ambient conditions and for low temperatures on Day 1 are highly desirable. Addition of a second test station for high pressure and other studies is worthwhile if external funding is attracted to support this. The external funding should also cover a significant part of any additional instrument build costs to allow provision for the second sample station.

The priority for initial upgrades will be to complete the detector coverage if this is not possible during the initial build. Further SE's could then be added.

Summary STAP recommendations

- STAP strongly endorses the science case with emphasis on high resolution powder diffraction ($\Delta d/d = 2.8 \times 10^{-4}$ at long wavelengths).
- T0 chopper recommended.
- High efficiency detectors (e.g. 12-layer B-10) are recommended with 1sr coverage as a bare minimum and preferably more to ensure "early success". Prioritise backscattering and 90 deg. detectors. Aim to increase to ~4-6 sr coverage as soon as possible.

- Focus on powder diffraction, with PDF and single crystals as desirable secondary activities. SANS (forward scattering detector), polarisation are lower priority.
- Second sample station is supported if external funds can be raised (e.g. for high pressure) – these funds should also contribute to the resulting costs of modifying shielding etc.
- Consider removal of air scattering especially for small samples, and having sample changers for ambient conditions and for low temperatures
- Progress on 2D Rietveld and other data analysis is very encouraging and should be continued (externally)

MAGIC

Science case

The science case of MAGIC remains very close to the case made in the proposal and endorsed by STAP and SAC: a focus on magnetism and correlated electrons, addressing current questions in areas of unconventional superconductivity, spintronics, nano and molecular magnetism, spin liquids and ices, emergent spin-orbit coupled and topological states, multifunctional materials and maintaining flexibility to address future questions emerging in the field. Many of the questions to be addressed benefit heavily from or even require polarized neutrons, which therefore is an indispensable part of the MAGIC design. The "full scope" version of the instrument will be able to carry out the whole science case and like the SAC we are convinced that it will open up many new opportunities, attract a large user community, and be a highlight in the instrument suite of the ESS. The "baseline configuration" version to some extent would compromise the general performance and sample environment, and specifically omit beam-shaping at the sample position. Absence of beam-shaping would compromise parts of the science case, in particular questions involving long-periodic magnetic states (e.g. skyrmions and some multiferroics) and the study of very small samples (thin films, tiny crystals of novel materials, etc).

Technical Design

MAGIC is conceived as a bispectral, permanently polarized, single crystal diffractometer for studying magnetism. Its design is guided by the need to measure Bragg diffraction throughout reciprocal space using thermal neutrons, and diffuse scattering in a restricted portion of reciprocal space using cold neutrons. Furthermore, it is intended that the instrument can study very small samples. The design has several important elements for these purposes. The bispectral functionality is provided by a solid state bender which can be positioned to inject cold neutrons into the guide system, simultaneously polarizing them. The guide is long, with a kink, which serves to avoid line of sight and allows the positioning of the polarizer for thermal neutrons. Choppers for pulse shaping and background suppression are included. Two detectors are required, on one side a large one for the thermal neutron Bragg diffraction experiments, on the other a detector of restricted height behind a supermirror analyzer for the cold neutron diffuse scattering experiments. Some further optional components are part of the design. These are a slit system for divergence control to allow excellent wavevector resolution for studies of long-period order (e.g. skyrmion materials), and a focusing device for studying very small samples. MAGIC has considerable shielding requirements - the cave is very large. The size seems not to be a problem – a smaller cave would be roughly as expensive and heavy, as thicker walls would be required. However, a roof is planned, which adds significantly to the cost and penalizes the budget accordingly. Accurate shielding calculation and costing is urgently required.

STAP comments

STAP noted that the science case is centred on frontier areas of magnetism and will remain relevant over coming years. Polarization of both cold and thermal beams, and with full XYZ analysis of scattered cold neutrons is essential to the science programme. The ability to study very small samples is world-beating and should be available from Day 1.

The design is mature and options have been considered carefully. STAP felt that it is important to accept the baseline configuration and add collimation and focussing options for beam shaping optics to enable small samples to be studied from Day 1. Having 60 out of 160 deg. of large detector coverage for the thermal beam is acceptable for initial performance. Provision of SE's including magnetic fields up to at least 10 T and dilution fridges is important. If these are not affordable from the initial instrument budget then other options within and outwith ESS should be explored (see General Comments). Options for cost reductions for the shielding and sample cave (but without compromising safety) could be explored (see General Comments).

Upgrade options should be to complete the large detector coverage if this is not possible during the initial build, and then to add dedicated magnets and fridges. Inclusion of a high field (60 T) magnet should remain a longer term aspiration.

Summary STAP recommendations

- We strongly endorse the science case, with full polarisation of thermal and cold neutrons.
- Small samples are important and therefore collimator and focussing for beam shaping are essential.
- SE are highly important and various routes should be considered; sharing; external collaboration, loans, donations.
- No reduction of baseline specification.
- Consider smaller/standardised cave.

HEIMDAL

Science case

The essential point of the HEIMDAL design is the combination of neutron powder diffraction (NPD) and small angle neutron scattering (SANS) and even neutron imaging. By providing separate guides for the cold and thermal neutron spectra the NPD and SANS experiments both receive a separate beam optimized to the specific requirements, rather than finding a compromise that uses a single common guide. The excellent time resolution will enable HEIMDAL to investigate reactions in real time. An essential aspect is the ability to investigate the wide range of length scales simultaneously in a single experiment. This can be applied to the formation process of many different functional materials. Examples are the formation of nanoparticles with a solution or within a host matrix, heterogeneous catalysis, or the formation of cementitious phases. A full understanding of these reactions requires us to understand the initial, intermediate and final phases at the local atomic level by powder diffraction. The characterisation of the resulting and changing cluster and pore shapes and sizes requires simultaneous SANS and large scale features such as grain sizes require neutron imaging. Thus HEIMDAL will offer unique experimental opportunities for light element materials and magnetic materials that are not suited for high energy x-ray diffraction.

Technical Design

The requirement of the science case for HEIMDAL to probe the structural properties of materials over an extended range of length scales requires a novel instrument design, which is significantly more complex (and potentially, therefore, more costly) than any currently available facility. Thermal and cold neutrons are transported to the sample position using separate curved guides. Unfortunately, changes to the design of the “butterfly” moderator design made by the ESS, including the possibility to dispense with the lower moderator, have hampered the design team’s ability to optimise the guide geometry. A number of choppers are situated in both guides, including a pulse-shaping chopper to provide improved $\Delta d/d$ resolution for the thermal neutron powder diffraction studies, and further choppers to define the wavelength range and eliminate frame overlap for both the diffraction and SANS measurements. A wide angle detector array is proposed for the diffraction studies, which can be performed simultaneously with SANS measurements using detectors located at relatively long distances behind the sample. There is also provision for a camera to be inserted downstream of the sample position, to provide imaging capabilities (including time-of-flight discrimination for Bragg-edge imaging methods).

STAP comments

STAP felt that the science case remains highly topical and relevant. HEIMDAL provides ESS and the international community with an adventurous novel instrument, driven by user community interests. The key novel and world-unique attribute of HEIMDAL is the use of separate thermal and cold neutron beams to respectively collect rapid NPD and SANS data. This will enable complex and changing systems to be studied over multiple length scales. STAP appreciates that the build will be expensive and therefore recommends a staged construction with a minimum requirement for Day 1 to have a working NPD diffractometer with a SANS upgrade path already defined. This interim configuration of HEIMDAL will complement DREAM in providing fast data collection for kinetic and parametric studies, enabling very small samples to be studied, and developing techniques such stroboscopic experiments and Bragg-edge imaging which will be important capabilities for the eventual full instrument. STAP noted that the project design has been delayed and is not yet mature. Immediate and continuing support from ESS is needed to bring HEIMDAL back on schedule.

The upgrade path to add SANS capabilities might attract support from relevant industries in partner countries. Imaging is a further, relatively inexpensive option to be added when funds allow. An imaging camera might be 'borrowed' from or shared with other instruments (e.g. the ODIN beamline?) in the meantime.

Summary STAP recommendations

- Science case is strongly endorsed with emphasis on simultaneous NPD + SANS (+ imaging).
- HEIMDAL reflects ESS desire for adventurous novel instruments, driven by user community.
- NPD with realistic SANS upgrade path is a minimum requirement (can industry contribute?).
- NPD programme will complement DREAM.
- Short term support and growth of instrument team is critical
- Explore the possibility of 'borrowing' an imaging camera from elsewhere (e.g. the ODIN beamline?)

GENERAL COMMENTS

Over the course of STAP discussions, several more general themes emerged and are reported here as comments for ESS to consider;

- Instrument teams often seem to be dealing with the same design issues in parallel. This potentially leads to wasteful duplication of effort, and perhaps in an overly complex ESS infrastructure. Standardisation of shielding, caves, services and other aspects of instrument design across all teams might lead to optimal designs and efficiency savings.
- Staff requirements are a significant fraction of all beamline construction projects. STAP wondered whether delaying appointments and sharing staff across instrument projects could lead to some savings.
- Overlap between horizontal and vertical STAPs and ESS teams is important to ensure efficient communications between all stakeholders.
- SE's are essential to the Day 1 programmes of many instruments but are at risk of being omitted from baseline specifications due to budgetary pressures. As well as providing optimal SE coverage in house, it is likely that ESS can benefit from community contributions and goodwill. For example, collaborations may be used to develop SE's during commissioning, and existing equipment may be loaned or donated to ESS.
- Similar opportunities to develop software for data analysis are likely to exist outside ESS with benefit from community contributions and goodwill, as illustrated by the recent demonstration of 2D Rietveld analysis of simulated DREAM data.
- STAP observes that the ESS Diffraction suite of DREAM, MAGIC, and HEIMDAL, as well as NMX and other instruments providing diffraction capabilities, will offer outstanding opportunities to the user community. However, there are still significant gaps to be filled, most notably in high pressure neutron diffraction where the cost-effective ESPRESSO proposal offering world-leading opportunities was recommended with equal priority to MAGIC by the 2015 STAP review.