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BEER – Initial Operation and Staging plan

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SUMMARY

The initial operations and staging plan describes the preliminary plan for the validation of the instrument function and scientific performance using spallation neutrons. This process is called "hot commissioning" and it is outside the scope of the instrument construction work-package. The document also describes the upgrades beyond the Day-one scope with final goal to reach Full scope configuration.

1. HOT COMMISSIONING

The aim of the hot commissioning of an instrument refers to the testing and validation of the instrument using neutrons from the ESS target station. The first objective of the hot commissioning of BEER is to prepare the instrument for successful enrolment into the User Operations phase (Phase 6 [1], early 2023) by validating various instrument functions and components. During the scope setting meeting for BEER, the basic version of the instrument, called Day-one scope (still competitive configuration), with for example a partial detector coverage (only two ±90° detectors), reduced chopper (5 choppers from 10 in total) and positioning (without heavy z-axis and small x, y, z tables) system and other downgrades, was accepted to move forward into detailed design and construction phases [1][3]. An upgrade path to the Full scope configuration will be realized through a staging process partially supported by the operational budget of the ESS and other external sources. Thus, the second objective of the hot commissioning is to demonstrate the instrument capabilities at Day-one but also to give hints of the performance of the Full scope configuration. That includes measuring challenging samples using complex sample environment, show the maturity of novel modulation technique for the fast high-resolution strain scanning and highlight the new approach of sample environment driven experiments. These two objectives of hot commissioning have very different requirements for the samples on the one hand and beam stability on the other. In this preliminary plan the two objectives will therefore be discussed separately, bearing in mind that the successful completion of the first is a necessary prerequisite for the second.

1.1 Validating instrument functions

A neutron scattering instrument is a complex system with many custom-built subsystems (e.g. optical system, detector system), consisting of a number of technical components (e.g. guides, choppers, detector units, electronic control units). The factory acceptance tests, installation and ESS acceptance tests of each individual component are part of the cold commissioning phase called, Phase 4 – Installation & Integration [1], of the instrument, but their function together as a system to perform scientific experiments can only be tested with neutrons. The goal of the function validation of the individual systems is to establish the readiness of the instrument to produce reliable experimental data. The validation of the instrument function starts with the validation of the neutron beam characteristics, essentially verifying that the functional requirements [4] have been met. The second part of the instrument function validation is data collection from a well characterized sample with known crystal structure, such as a NIST Si standard, Ni, diamond, Al_2O_3 and NAC ($Na_2Ca_3Al_2F_{14}$). Strain scanning measurement and data evaluation of already characterized samples and published data will be used for validation of the instrument capabilities in strain mode.

1.1.1 Instrument shielding Validation

The Neutron Optics and Shielding group (NOSG) will provide guidelines and assistance in measuring shielding characteristics in the point of radiation doses along whole instrument. The NOSG will provide a detailed plan and schedule for shielding characterization necessary for the hot commissioning phase and licencing.

1.1.2 Neutron Beam Validation

The beam monitor in the experimental cave provides a relative measure of the beam intensity as a function of the time-of-flight (TOF). The neutron flux at the sample position will be measured with the flux measurement assembly. The beam divergence and size at the sample position will be measured with the beam visualization system. The pulse length at various wavelengths will be measured using an inorganic crystal of known mosaicity. Measurements of the various types of unwanted radiation (gamma rays, fast neutrons, thermal neutrons outside the desired bandwidth) will be made when necessary by the instrument team or appropriate ESS technical groups.

1.1.3 Data collection from standard samples

The objective of this part of the hot commissioning is to verify beyond any reasonable doubt that the instrument is ready for the data collection. The powders which are deemed to be calibration standards in powder diffraction (Si, Ni, diamond and NAC) will be purchased from National Institute of Standards and Technology (NIST). In addition, solid rod of vanadium of various diameters, corresponding to the size of sample holders will be obtained. For validating strain measurements capabilities of BEER a suitable define-strained sample will be used. All of the powder samples have been previously characterized at other diffractometers around the world. Therefore, such important characteristics of the BEER instrument as resolution, peak profile, peak position and signal-to-background ratio can be directly compared with existing instruments at other facilities. A powder reference measurement will also allow for checking systematically the various TOF resolution settings that will be possible with the pulse shaping or modulation chopper system. Adjustment of the data reduction routine for the modulation technique will be made. The data analysis within standard Rietveld and 2D Rietveld refinements will be done to obtain the crystal structures or individual reflection characteristics of all samples. The quality of the fits and standard deviations in refined parameters will allow us to benchmark BEER with other instruments, particularly in terms of counting time and minimum amount of sample needed to obtain refinable patterns or reflection profiles at various high flux/high resolution settings. The advantage of 2D Rietveld refinements and modulation technique will be emphasized as well.

Installation and easy integration of different sample environments is crucial for the BEER instrument work flow. Different modes of experimental control using available SE will be tested. Proper time stamping of SE status signals and reduced data binning will be monitored to properly bind those data and produce meaningful experimental output.

During the hot commissioning “friendly” (i.e. experienced) users will be admitted to the instrument to measure actual samples relevant to their research agenda. It will help to identify potential issues with the data accessibility and measuring modes of the instrument. At the same time, successful user experiments at early stage of hot commissioning will help to promote the instrument and make it appealing for a wider user community. A positive word-of-mouth in the early days of instrument operation is critical for its long-term success. For this purpose the flag-ship experiments for each instrument modality [5] available at Day-one will be designed and realized during hot commissioning.

After a successful data collection on standard and actual “friendly” user’s samples, the instrument is in principle ready to enter the general user program, provided that all the requirements related to instrument operation [4] have been met.

2. STAGING PLAN FOR THE FULL SCOPE INSTRUMENT

2.1 Staging plan for Instrument

The Day-one scope of the BEER Instrument Construction Work Package will deliver a functional instrument with a competitive performance within the overall budget of 14.987 M€, agreed upon during Scope Setting meeting [3]. A contingency of 1.32 M€ (~10%) is included into this budget. The performance and throughput of the instrument could be significantly increased by upgrades, which are outlined below.

The upgrade of the instrument to the Full scope should extent the instrument equipment by additional choppers, positioning system, detector coverage and SANS detector. There are also other smaller upgrades which are foreseen as is described in the proposal [6]. These upgrades will increase the instrument capabilities by adding options for higher flux (shorter measurement times) ([5], HLSR 2.-4. and Chapter 7). It will also enable new experiments which require simultaneous measurements with thermal neutrons (diffraction) and cold neutrons (SANS or imaging) by additional chopper operation modes and by installation of the SANS detector ([5], HLSR 4., 14. and Chapter 7).

A list of items scheduled for the BEER staging ordered by priority with draft schedule and expected cost is given in Table 1. Detailed description of each item is made in following chapters.

Cold and hot commissioning will be needed after installation of each item. The instrument control software needs to be designed so that accommodation of new parts is easy. BEER concept has been developed having the Full-scope setup in mind, which should make integration of new components during staging easier.

Table 1 - Items of BEER upgrade staging with drat schedule and cost estimate.

Priority	Item	Schedule	Cost (k€)
1	3rd PSC chopper	Q2/2022	191.55
2	2nd modulation chopper	Q3/2022	206.55
3	3rd FC chopper	Q4/2022	176.55
4	4th FC chopper	Q4/2022	176.55
5	Linear stages	Q1/2023	30
6	Laser tracking system	Q1/2023	100
7	Detectors at 130°	Q2/2023	1202.45
8	Horizontally focusing guide stage	Q3/2023	110
9	Back scattering detector	Q4/2023	707.25
10	Heavy z-axis table	Q1/2024	200
11	Off plane detectors	Q1/2024	2719.9
12	Detector at 50°	Q3/2024	1202.45
13	SANS option	Q3/2025	1399
14	3rd modulation chopper	Q3/2025	176.55

2.1.1 3rd PSC chopper

This chopper is placed in the chopper casemate just after the monolith wall. It is a fixed chopper which is designed to allow together with the first PSC chopper the high flux option with relaxed resolution. Installation of this chopper should be done as the first upgrade because the high flux option will be needed to reach short measurement times required during real time dynamical in-situ experiments. This upgrade increases the range of resolution / flux options that can be offered to the users, making BEER even more flexible than other engineering diffractometers.

The common chopper CHIM holding the PSC choppers will be designed in such a way that the installation of 3rd PSC chopper could be done remotely (operation already after the first proton on target). Installation should constitute of removing the dummy plug and placement and adjustment of the chopper body.

2.1.2 3rd and 4th FC chopper

Installation of these choppers, which should be done at once, helps to increase the variability of the possible operation modes available for the BEER instrument, especially the usage of double frame option or alternating frame option which can be used for extending the wavelength ranges used for the experiments.

3rd FC chopper is located in the same chopper housing as 1st FC chopper (face to face choppers) at the distance of about 8.3 m from the source. The housing will be designed to enable the installation of a second disc. The CHIM system on the other hand allows the extraction and installation of the chopper system remotely (operation already after the first proton on target).

4th FC chopper is situated in the same housing as 2nd FC chopper (face to face choppers) at the distance of 80 m from the target. The chopper system is outside the bunker area, which makes the installation easier without necessity of remote handling. The chopper system (housing, CHIM, …) will be designed to make placement of the chopper easy.

2.1.3 2nd modulation chopper

The second modulation chopper will share housing with the first one at 9 m (face to face choppers). It is needed for better usage of the modulation technique, especially to increase the distance between multiplexed reflections.

The housing will be designed to host a second disc and the common CHIM will be designed to enable the installation of the chopper system remotely (operation already after the first proton on target).

After this upgrade the chopper system will be completed for the diffraction options and BEER will have all the diffraction modes as proposed in the proposal [6]. One more modulation chopper disc is used in case of simultaneous Diffraction and SANS measurements.

2.1.4 Linear stages and laser tracking system

To increase the sample manipulating capacity of the instrument the additional x, y and z tables will be installed. Those tables will provide faster and easier adjustment of positioning of small samples for strain scanning or automatic sample exchanging system. Furthermore they provide longer travelling distances compared to the hexapod.

A laser tracking system will be used to increase the precision of the sample positioning systems (robot, hexapod, linear stages, etc.). This is needed for better reliability of the strain scanning of complex shape and heavy samples, alignment of big SEs or long term experiments platforms.

2.1.5 Additional detectors

Installation of the additional in-plane detectors increase the instrument performance for data analysis of multi-phase samples, coverage for texture analysis and throughput due to the higher detector coverage. There is a plan to have two additional 1x1 m^2 detectors at 50 and 130°C of 2θ. And then one smaller 0.5x0.5 m^2 high resolution back-scattering detector at 165°.

The detector technology used for those additional detectors will be the same as for the Day-one detectors. The very similar detectors support as for the ±90° detectors will be used. Time schedules of each detector including the cost estimate are shown in the Table 1.

2.1.6 Heavy z-axis table

The central sample table will be equipped from Day-one with only rotational table and additional positioning system what limits the alignment of heavy samples and equipment along the z-axis. To enable this possibility the heavy z-axis table to be able to handle 3 ton samples will be installed bellow the rotation table to complete the sample tower.

To install this table a reconstruction of the sample stage will be needed – replacing of the support of the rotation table. The sample tower shaft in the floor platform will be designed to enable this installation and future maintenance of the stage.

2.1.7 Off-plane detectors

The off-plane detectors will increase the performance of the instrument in the point of in-situ texture evolution and rotation-less texture analysis. Off-plane detectors should cover angle about 100° out of the horizontal diffraction plane. This option makes the instrument very powerful and demanding for the engineering community dealing with material processing.

Detector technology of the off-plane detectors is planned to be the same as for the in-plane detectors. A stable construction holding the off-plane detectors will be designed with spatial and stability restrictions what this option imposes.

2.1.8 SANS option

SANS option is planned as the last upgrade option. This consists of two parts. The first part is the installation of the 3rd modulation chopper at distance of 9.5 m from the target. The installation of this chopper system needs to be done remotely (after the first proton on target). In the guide design of the Day-one configuration the later installation of this chopper system is already foreseen.

The second part consists of the installation of the vacuum tube and movable detector inside the tube. Installation of the big vacuum tube will need to be done throughout the roof. This makes the installation quite difficult and time consuming and should be planned for the long shutdown. Technology for the SANS detector can be selected later based on experience from other SANS instruments or experience with other technologies.

2.2 Staging Plan for Sample Environment Equipment

One of the main goals of the BEER instrument is in-situ experiments which need dedicated sample environment. Pool SE will also be possible to use. Due to the reduced scope, all of the BEER-specific SEs were removed from the Day-one budget, indicating that external funding opportunities need to be found or an application for financial support from the operational budget need to be made. After BEER scope setting meeting the SAC advised to increase the budget of the SAD group to cover the two important SE from the BEER suite – dilatometer and the stir-wielding machine. Those will be designed, procured and installed by SAD but with strong assistance by the BEER team. The advanced deformation rig, one of the main SE, will be most probably designed and constructed from the Swedish government funds in collaboration with Swedish universities representing engineering user community. If those projects are not funded, re-examination of the instrument budget [3] or another solution need to be considered.

The deformation rig should be available on Day-one when hot-commissioning period starts. It will be used for the first experiments which prove the concept of the instrument and demonstrate its capabilities to the user community. The deformation rig is therefore very important for early success of the instrument. Other two SE paid from SAD budget – dilatometer and stir-welding – should be available during the hot-commissioning period as is noted in the Table 2. In Table 2, there are also other SEs (coloured) foreseen for the future upgrade period together with their schedule and expected cost. Those SE will be funded from external sources, mainly projects of collaboration with universities and other research institutions. They are shown here just to illustrate the instruments team plans towards the user community.

Table 2 - Items of SE staging of BEER instrument including draft schedule of installation and cost estimate.

Priority	Item	Schedule	Cost (k€)
1	Advanced deformation rig	Q4/2021	in-kind*
2	Dilatometer	Q2/2022	SAD
3	Stir-welding	Q1/2023	SAD
4	Bi-axial stress rig	Q2/2024	400
5	Digital correlation system	Q3/2025	100
6	Annealing furnaces	Q3/2024	50
7	Laser welding machine	Q4/2026	200
8	Gleeble® simulator**	Q1/2028	2000

* - Swedish government funds in collaboration with Swedish universities; ** - external funding needed; [coloured] - not part of the staging process

The priority of each SE or definition of new SE can change in the future depending on the user's requirements and funding option availability.

Each SE will be seen as individual project with their phases as described in [1]. Interactions with SAD staff during all phases of the project will be needed. The instrument dedicated SE might be commissioned with a minimum input from SAD, while SE paid by SAD or pool SEE will require full support of SAD staff. During the installation and integration of each SE we suppose close collaboration with the SAD staff.

3. GLOSSARY

Abbreviation	Explanation of abbreviation
BEER	Beamline for European materials Engineering Research
CHIM	Chopper mechanical Integration Module
FC	Frame selection Chopper
HLSR	High Level Scientific Requirements

Abbreviation	Explanation of abbreviation
NAC	$Na_2Ca_3Al_2F_{14}$
NIST	National Institute of Standards and Technology
NOSG	Neutron Optics and Shielding Group
PCS	Pulse Chapping Chopper
SAC	Scientific Advisory Council
SAD	Scientific Activities Division
SE	Sample environment
TOF	Time-Of-Flight

4. REFERENCES

[1] Process for Neutron Instrument Design and Construction (ESS-0051706)
[2] Scope Setting Report Instrument: Engineering Diffractometer BEER
[3] Summary of BEER Scope-Setting
[4] BEER – System Requirements Document
[5] BEER – Concept of Operation Description
[6] ESS Instrument Construction Proposal <<Beamline for European materials Engineering Research (BEER)>>

DOCUMENT REVISION HISTORY

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