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BEER - Concepts of Operations Description

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1. INTRODUCTION

The purpose of this Concept of Operation document, ConOps, is to provide a brief description of the BEER instrument, Beamline for European materials Engineering Research, and in particular its basic concepts in the Day-one configuration. The changes foreseen due to the upgrade to the Full-scope instrument are discussed in a separate chapter at the end of the document. The Day-one configuration means the instrument agreed after the scope-setting meeting [1][2] which represent reduced performance due to the budget restrictions and which will be designed in such a way to be easily upgradable into its full-scope as described in the proposal [3]. The document includes high-level scientific requirements, description of individual parts of the instrument in the context within which the instrument will be designed and constructed as well as the main modes in which the instrument will be operated. All these are placed within the framework of the instrument life-cycle.

The intended audience for this document includes everyone involved in the construction and operation of BEER, i.e. all central stakeholders. It will also serve as a quick overview of the instrument's purpose, construction and operation for both persons familiar with the field of neutron science, neutron engineering diffraction in particular, and those that are not. The ConOps is intended to be updated several times to ensure its actuality.

2. HIGH-LEVEL SCIENTIFIC REQUIREMENTS

Scientific requirements for the Day-one scope are a subset of the requirements of the Full-scope and both are based on the science case depicted in the instrument proposal [3]. The science case of the instrument BEER can be summarised into four modalities which will be supported by the instrument. The Day-one scope is designed to allow most of the modalities in a reduced scale but with an easy upgrade path to full scope capabilities. Description of the process and time schedule of the staging process from the Day-one scope to full one are described in the Initial Operation and Staging plan document [4].

2.1 Instrument modalities

High-level scientific requirements are based on the science case and the necessity of high performance and flexibility to exploit the specific strength of the long ESS pulse. The instrument dedicated to the materials engineering research, as the BEER instrument will be, need to be able to accommodate new trends in the materials research as well as to support common approaches. The scientific requirements need to underline all the modalities which will be supported by BEER and these modalities can be summarized as following:

I. **In-situ & in-operando experiments** under real engineering conditions with time resolution below 1 second and with the ability to resolve nuclear and/or magnetic structures of multi-phase materials together with its microstructure. *Reason:* Materials for engineering applications are becoming more and more complex. Developments of multi-phase systems with complex microstructures need multi-scale characterization techniques and knowledge of processes taking place during manufacturing to tailor desired properties. In the real manufacturing situation, subsequent processing steps follow in very fast time regime (sub-seconds) to cope for a high through-put in short production time in large scale industry machines. The high intensity of the ESS source in combination with a tunable time structure of the pulse allows a quick collection of structural (nuclear and/or magnetic) and microstructural data using even complex sample environments within a short time period. To push further a technique in-situ

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experiments based on the passive characterization, where sample environment procedure is designed before and fixed during the experiment, an active in-situ material processing based on the real-time changes is envisaged. To actively tailor material properties based on the structural and/or microstructural characteristic, the real in-situ information and adaptation of thermo-mechanical process is needed. This can be achieved by interactive feedback control from a real-time data analysis of the scattering data. Other aspect of the new experiment control approach is the response to a temporary source failure. For some processes, it is essential to follow a prescribed schedule of cooling/heating, dwells on temperature etc. In standard instrument control approach, this schedule is interrupted, which brings the material to the state which was not foreseen by the initial plan. To avoid this problem, another option is suggested, when the thermo-mechanical process continues without neutrons as planned, and the neutron measurement restarts as soon as the beam is again available. This increases the robustness of the instrument and user time usage.

II. **Strain scanning** with a higher throughput. *Reason:* The strain scanning technique is a well-established technique used by material engineers to reveal the internal stresses within real-shape samples. With the more complex sample shapes, there is an increased demand for the strain mapping from large sample volumes and also larger depths. Due to a unique modulation technique developed to enhance the usage of neutrons from the long ESS pulse, it will be possible to speed up the strain scanning technique or to reach larger depth for highly symmetric materials by order of magnitude. By using an advantage of time-of-flight technique and two detectors positioned at ±90°, it will be possible to measure two strain components at once. Advanced positioning systems combined with 3D sample scanning will enable reconstruction of the strain maps even for complex shape samples.

III. **Texture and texture evolution** measurements during in-situ experiments. *Reason:* Evolution of the textures during a mechanical load or a thermo-mechanical treatment allow for observation of reorientation of the microcrystalline ensemble i.e. micro crystals in advanced engineering materials which define global material properties such as fracture strength, fracture evolution, etc. To enable this option, the high brightness source, low background, and off-plane detector coverage are needed. With sufficient high resolution provided and big detector coverage will be possible to follow the texture changes for individual phases and/or grains what is very important in large grained materials as rocks or annealed alloys to predict their bulk properties. The capability for texture measurements is limited in the Day-one configuration of BEER due to reduced detector coverage but will improve by staging to the Full scope configuration of BEER.

IV. **Long-term experiments** studying slow engineering processes (fatigue, corrosion, creep) which cannot be completed during one beamtime slot allocated to the experiment. *Reason:* Non-destructive structural and microstructural analysis of the slow processes in-situ is very useful to understand processes taking place within the materials. Such experiments may require periodical measurements of the same sample on the neutron beam over a long time (weeks to months). This requires running of the material experiment out of the beam and its occasional transport to/from the neutron beam. The engineering laboratory available for BEER will enable not only the preparation of experiments with complex sample environments but also offers a storage space for long-term experiments which will need only occasional measurements in the beam. A universal platform for transport and docking of such

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experiments, where samples will be pre-aligned, helps with precise positioning in the beam what is crucial for data analysis.

To fulfil these modalities of BEER, the high-level scientific requirements are expressed as follows for the Day-one scope.

2.2 Day-one scientific requirements

1. BEER shall allow the measurement of structural data of engineering materials (e.g. duplex-steel) in the form of determination of cell parameters with accuracy of $\Delta a/a \sim 10^{-5}$. (I, II, III, IV)
2. BEER shall accommodate all possible sample environments that will satisfy the science case especially the collection of scattering data for in-situ and in-operando experiments. (I, III, IV)
3. BEER shall allow the scanning of residual strains of minimum value of 50 µstrain on samples with complex shape as 150 mm diameter, 10 mm wall thickness tube in a time frame comparable with existing instruments. (II)
4. BEER shall allow the measurement of type 2 & type 3 strains and texture. (I, III, IV)
5. The experimental cave design of BEER as well as the design of the adjacent laboratory shall allow the access-on-the-beam of ex-situ-running long-term experiments for occasional measurement. (IV).
6. The detector coverage together with the available wavelength bandwidth shall be optimized for a sufficient d-range for common engineering materials which is identified as 1 - 3 Å. (I, II, III, IV)
7. The instrument shall allow measurements of two strain components at once. (II)
8. BEER shall allow the gauge volume to be adjusted for the experiment down to about 1 mm^3. (I, II, III, IV)
9. BEER shall allow data to be collected to d_{min} of about 0.7 Å for detectors at 90°. (I, II, III, IV)
10. BEER shall allow d-resolution ($\Delta d/d$) to be optimized for the experiment ($0.1\% < \Delta d/d < 0.3\ \%$) by trading intensity for resolution. (I, II, III, IV)

The requirements 8 and 9 are outside the scope of the BEER construction project but constitute important requirements for the science case. Here BEER is dependent on its scientific requirements on the project of the DMSC with which it has correspondingly an important interface where such specific requirements have to be communicated and implemented.

3. SYSTEM CHARACTERISTICS

3.1 System purpose

BEER is a neutron diffractometer addressing the needs of material engineers to characterise bulk structures, microstructures, and/or stress states of advanced materials for engineering and industrial applications. The instrument concept is optimised in its full-scope for in-situ and in-operando experiments under thermal and mechanical conditions similar to those in real industrial processing and use. So the way how to control the instrument is based on the new

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approach when an experiment is driven by a sample environment, not by the diffractometer. Thermo-mechanical data collected during a complex thermo-mechanical experiment are very important, but there is a lack of the equally important information about the crystal structure and microstructure, which could be directly linked to the same macroscopic state of the same sample. The purpose of BEER is to provide this structural and microstructural information during in-situ and in-operando experiments. An active feedback when a thermo-mechanical procedure is modified during the experiment by an algorithm based on real-time analysis of scattering data is envisaged, and it will move the engineering diffraction experiments to a higher level. One of the key components of BEER in its full-scope is, therefore, the sample environment. BEER allows the usage of advanced sample environments for simulation of different kinds of engineering processes simultaneously with the measurement of structural (diffraction) data.

Well established engineering diffraction techniques to analyse the residual stresses in real shaped samples will also be feasible within the BEER instrument. The design of the sample handling will allow using 3D models of the sample for positioning within sample coordinates what makes then reconstruction of 3D residual strain maps easier. The data collection can be largely enhanced by employing the long pulse of the ESS together with the modulation technique.

Infrastructure for carrying out accompanying ex-situ material testing including long-term experiments and proximity of the support laboratory for materials engineering are essential for successful operation of the instrument.

3.2 High-level system requirement

In order to achieve those high-level scientific requirements and to support the depicted modalities and the science case in taking the best advantages of the ESS long pulse source following high-level system requirements have to be met. Those are core design requirements, beside the other functional requirements listed in the corresponding document [5], which address basic requirements for neutron engineering diffractometer (high-intensity/high-resolution modes, two 90° detectors, …), but also BEER specific requirements coming from the science case needs and they can be summarized as follows:

- The SANS measurements in the Full scope configuration and Bragg edge imaging will require access to high wavelength neutrons above 3 Å with sufficient intensity what implies the necessity of using a bi-spectral extraction system allowing to combine both thermal and cold neutrons in the neutron guide system.
- The analysis of multi-phase systems and variability of modalities will need a tunable intensity/resolution and bandwidth centre wavelength. So a complex chopper system which can shape the source pulse as needed is required.
- The high-resolution $\Delta d/d$ of 0.14% at 90° detector with distance from sample 2 m requires horizontal resolution of the detectors to be at least 2 mm.
- The envisaged modulation technique for fast data acquisition for highly symmetric materials will need special modulation choppers and software enable to simulate Bragg reflection multiplication based on the structure and help to predict appropriate chopper settings.
- The modulation technique will require special data reduction routine and precise chopper phase information.

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- Measurement of two strain components at once requires high detector coverage at least at ±90°.
- From the active-feedback experiment-control follows the requirement of fast data acquisition, reduction and analysis software which need to be robust and easily configurable.
- All in-situ experiments will require sample environment which needs to be easily transported in and out of the experimental cave. The sample environment requires a platform for external alignment and processing as well as readiness at the instrument plug-and-play connection. Storage for not used sample environment will be required.
- Strain scanning experiments will require the 3D scanning tools and advanced positioning system which enable precise manipulating of the sample.
- Long-term experiments will require access to the engineering laboratory where they can be operated and from which they can be transferred for occasional measurement.

Some of the system requirements contain the items not directly related to the BEER project but with the DMSC project what makes it an important interface. We found useful to state it here because it gives a better overview of this interface and interlink with a specific part of the BEER project.

3.3 System Lifecycle

Figure 1 shows the life-cycle of the BEER instrument on a high level, schematically and without the details of the corresponding further detailed development phases. Each phase of the instrument development is concluded with a TG review, with accompanying design review.

The schematic process below is a simplified depiction as in reality there are overlaps needed between the seemingly separated phases. The most time important items as a guide, choppers, shielding need to start with procurement and manufacturing before proper TG review will take place with approval by ESS. The Instrument Development process provides the framework within which the instrument will be developed with timely milestones in order to measure progress, still allowing for an overlap to exist. The controlling document for the instrument development is Process for Neutron Instrument Design and Construction [6].

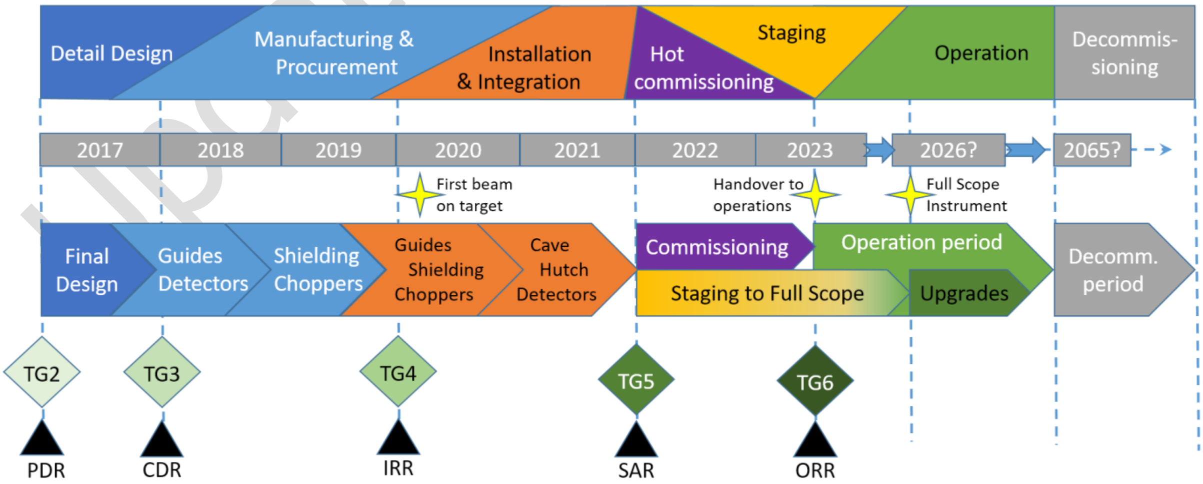

Figure 1: Schematic Instrument Development process and its relative life-cycle

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The Scope setting meeting described the instrument scope which needs to be delivered in the construction phase which ends by reaching TG5. After TG5, there is a procedure called "Staging to full scope" where the Day-one scope instrument is continuously upgraded to the Full one which is described in the instrument proposal [3]. The Day-one scope of the instrument is designed and constructed in a way to meet three criteria:

1) Realise the project within the agreed budget (cost book value set throughout the scope setting process [2]).
2) Allow to be easily staged to the full scope.
3) Enable some of the unique features to highlight the necessity of the BEER instrument and its early success.

Description of the Day-one scope together with the budget is done in the Scope Setting Report Instrument: Engineering Diffractometer BEER [1] with adaptation according to Summary of BEER Scope-Setting [2].

It is however currently unclear when budget security can be achieved for a staging process towards the full-scope. This also makes unclear the date of the final commissioning. We suppose that the instrument can be shifted to the operations before the full-scope is reached as it is reflected in Figure 1. Description of expected prioritisation and draft time planning for the staging process are described in more detail in the chapter 3.4.12 on page 14 hence the external documents mentioned in that chapter.

The decommissioning efforts depend strongly on the exposure time of each component within the radiation environment and its composition with respect to easily activated elements. For beamline components which can be exposed to a direct or scattered beam, materials with low activation elements are foreseen to minimise the decommissioning efforts.

3.4 System Overview

3.4.1 General

The conceptual design of the BEER instrument is subdivided into the following generic main functional blocks:

- Neutron optics system
- Shielding
- Chopper system
- Shutters
- Experimental cave
- Sample exposure system
- Detectors and monitors
- Personnel Safety System
- Control hutch
- Instrument control

They have to be defined and designed in a way that fulfils the high-level requirements as the basis for the detailed functional and non-functional instrument and component requirements.

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Figure 2 shows a schematic drawing of the Full scope instrument layout with the main construction components, which are described in the following sections.

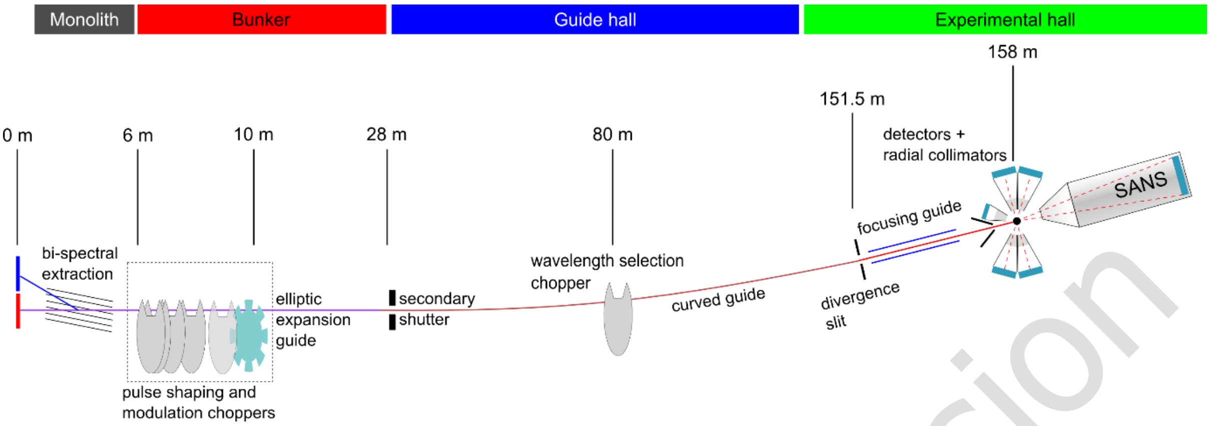

Figure 2: Schematic drawing of the BEER instrument layout with key components.

3.4.2 Neutron optics system

The neutron optics system has to fulfil the requirements concerning efficient neutron transport within the required wavelength ranges and adjustable divergence intervals, as well as the requirements on effective shielding, respecting all technical and cost constraints.

The whole neutron optics system can be, in the top level schema, divided into six main parts:

- *Neutron extraction system* – a neutron guide inserted in the monolith and light shutter. Its vertical profile follows an ellipse allowing for efficient extraction of neutrons from the 3 cm high top moderators. The neutron extraction system includes as well the multi-mirror extraction system to combine spectra from both the thermal and cold moderators which is located just after the light shutter.
- *Chopper sector* – the section between 6 m and 10 m from the source includes a cascade of choppers, which require a guide of reduced beam width (2 cm) with several gaps. Neutron guide segments in this sector have to be designed together with the chopper vacuum housing and maintenance system in order to ensure minimization of guide interruptions and the system robustness with respect to alignment accuracy.
- *Curved part* – after the chopper section the guide continue with the reduced beam width of 2 cm up to the bunker. The radius of curvature is -2 km what closes the direct line of sight to the source for the first time at the outside edge of the bunker wall.
- *Beam expansion part* – downstream from the bunker wall about 29 m from the source, the beam is horizontally expanded from 20 mm to 40 mm (elliptic guide profile) to allow for more efficient neutron transport to the experimental hall. This expansion section ends at 39 meters from the source.
- *Beam transport part* – a 105.5 m long guide (40x80 mm^2) curved to R = 20 km, which permits the direct line of sight to the source to be closed for the second time.
- *Focusing optics* – the last section starts at 13.5 m before the sample. It focusses the beam vertically and consists of three sections (lengths 7, 3.5 and 2 m), delivering at the sample the neutron beam of required maximum divergence (5 x 30 mrad^2). The last (2 m) section is exchangeable with an optional guide including horizontally focusing optics for high-flux measurements or with a simple vacuum tube (no guide) for high-

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resolution (low divergence) measurements. The divergence can be further restricted by two adjustable slits placed in between the last two sections. The third adjustable slit with variable distance has to be placed as close as possible to the sample in order to define the gauge volume size perpendicularly to the incident beam.

All these guide sections follow the same vertical ballistic profile, starting with an elliptic expansion part (distance 2 m to 15 m, height 35 mm to 80 mm) and ending with the above described focusing section (distance 144.5 to 158 m, height 80 mm to 30 mm).

3.4.3 Shielding

The instrument shielding consists of the guide shielding between the bunker and experimental hall, shielding of the experimental cave, and additional light shielding of components inside the cave, such as detectors and focusing guide, and a beam stopper. Its purpose is to limit the dose rate outside the shielded area and, if the beam is closed, also inside the experimental cave, under the limits imposed by safety regulations for surveyed zones. In addition, the shielding should protect other instruments with high background sensitivity from the noise generated by the neutron beam of BEER.

The shielding specification can only be defined on the basis of radiation transport simulations, which are currently under investigation. From the first simulation results of the shielding along the transport guide is evident that equivalent of less than 60 cm of heavy concrete (density 4.0 $g \cdot cm^{-3}$) will be sufficient to stop γ-radiation generated from the interactions of the neutrons with the guide coatings layer.

3.4.4 Shutters

To enable experiment preparation and sample exchange during standard ESS operation periods, a safety shutter is needed at a position after the first DLS closure, i.e. just after the bunker wall. This shutter needs to stop all radiation propagating downstream, especially high energy neutrons, in order to secure the radiation safety in the experimental cave. The shutter will also enable easier maintenance of the guides and the chopper placed after its position. The design will consider this shutter as safety shutter with an interaction to the PSS system.

3.4.5 Chopper system

The chopper system is a crucial part bringing to the instrument concept its enormous flexibility in the form of wavelength selection, tuneable resolution, time modulation, etc.

The choppers can be classified by their function into three categories (for more detail in [3]).

- PSC – pulse shaping choppers situated close to the source (see Figure 2) are required to tune $\Delta\lambda/\lambda$ resolution in the range suitable for diffraction. The concept of PSC choppers is based on disc chopper pairs operated in an optical blind mode. The PSC windows are chosen to allow for the maximum mean wavelength of about λ_{max}= 8 Å.
- FC – frame choppers are used for wavelength frame selection and to prevent undesired frame overlaps.
- MC – modulation choppers are used to create several short pulses out of the main ESS pulse, which are projected to the detector as several pulses with shifted wavelength. The multiplication factor can be tuned by the speed of the chopper. In the Day-one scope configuration of BEER, only one modulation chopper disk will be available in the chopper cave at about 9.3 m from the source.

All choppers, except one FC chopper at 80 m from the source, are situated within the bunker. This means that they will not be accessible for maintenance during the target operation. Due

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to this fact, low maintenance components are needed. The instrument can operate in certain modes without using some of the choppers (MC, PSC). To be able to operate the instruments in these cases or the case of chopper failures it is indispensable to unblock the neutron beam either by rotating the chopper disc to open positions or to remove the chopper out of the beam.

A straightforward and precise information about the phase of crucial chopper discs in addition to the time stamping system of the ESS high-speed data network will be used both for diagnostics and data analysis purposes. This solution is required by the complexity of the chopper cascade and the instrument dependency on the accurate knowledge of the time of flight especially when using the modulation technique. It will also increase the robustness of the system and permit measurement continuation in a case of temporary ESS data network failure.

3.4.6 Experimental cave

The experimental cave is a shielding construction enclosing the operational units for sample positioning and handling, detector systems, the end section of the focusing guide and apertures, a small crane for manipulation of large samples and sample environments. It will permit easy placement of large samples and sample environments and provide a suitable low gamma and neutron background for the best possible S/B ratio conditions for the large area detector systems.

The instrument cave will be situated in the experimental hall 3 (E01) where the floor level is 3.137 m bellow the beam centre line. To enable easy sample handling, it is foreseen that the cave will have an elevated floor of about 1.5 m from the hall floor. It is also foreseen to have two accesses to the cave: One big port with heavy doors for entering of the sample environments and big samples using a high-load lift, and the second entry for personal access through a chicane from shielding walls with a light lockable door.

Within the cave, there are requirements for access to various utilities like compressed air, gases, exhaust, electricity, etc.

The instrument cave, which will start at the inner wall of the experimental hall 3 (E01), needs enough space to host all detectors of the Full scope configuration including the SANS tube. It also should foresee space for the movement of detectors during installation of sample environment. The exact dimensions will have to be adapted to the requirements of the neighbouring instruments and free corridors to the guide hall. The height of the cave has to be chosen with the height of the experimental hall and crane access in mind as well as taking into account the weight and height of equipment that will be potentially added and removed through the ceiling.

3.4.7 Sample exposure systems

Several positioning systems are foreseen to be used to enable sample handling in different kind of experiments envisaged for the instrument.

The main positioning system will be designed in the form of a “sample tower” going through the elevated cave floor and consisting at Day-one of a full rotation table along the z-axis (perpendicular to the floor). Additional positioning systems will be placed on top of this main positioning system, depending on the experiment, which for example enable additional movements such as x, y and rotation stages, cradles, cybaman, etc.

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In addition to the sample tower, there will be a 6-axis robotic positioning system for strain scanning and texture measurements and a heavy load hexapod positioning system. Those systems will be removable and will be installed when required by the experiment.

3.4.8 Detectors

Detectors are a crucial part of the instrument. To fulfil the scientific requirements, two main detectors with the active surface of 1x1 m^2 ($28x28°^2$) and detection distance of 2 m from the sample, are foreseen. They will be placed at ±90°. The spatial resolution needs to be at least 2x5 mm^2 (horizontal x vertical). Several sets of radial collimators for different gauge widths will be necessary to provide suitable gauge volumes for various experiments. The detectors can be moved to and from the sample position along the radial axis to enable placement of large samples and sample environments on the sample position. A positioning system for precision tracking of the detectors placement is foreseen. The final solution is not yet fixed, but it can be built on already existing solutions to be used within the ESS [7].

These detectors should be based on detectors with $^{10}B_4C$ converter plate technology which is under development, but the first prototype was already tested and is available. These detectors would offer sufficient spatial (2x5 mm^2) and time (< 1 μs) resolution together with high quantum efficiency (60% at 2 Å). Backup solutions based on ^{3}He-tubes and scintillator technology are under investigation.

In the transmitted beam, a small (~40x40 mm^2) position-sensitive detector would serve to the imaging option, with the possibility of wavelength dependent analysis (Bragg edges). A CCD camera or an MEDIPIX/TIMEPIX based detector employing a microchannel plate converter/amplifier is considered as a suitable technology for this purpose. It is foreseen that this imaging option will be in early stages shared with the imaging instrument ODIN because this small detector is easily portable and can be transported between the instruments including analysing options.

A small neutron camera based on the scintillator technology is also envisaged for a sample alignment within closed sample environments.

2D sensitive transmission monitors placed close before sample and after the chopper systems allows for cross-checking of the chopper system operation and normalisation as well as the assessment of the incident beam on the sample.

3.4.9 Control hutch

A control hutch will host remote control equipment, computers, and the experimentalists. It is foreseen to have the control hutch as close as possible to the experimental cave to facilitate an access when adjusting the experimental setup. However, spatial constraints in the experimental hall probably force us to place the hutch on the 2nd floor, behind the experimental cave. The ground floor will be used for storage and potential off-beam operation of instrument-specific sample environment devices, such as furnaces, deformation rigs, cycling and creeping machines, as well as specialised devices like the Gleeble® simulator or a dilatometer. Life video surveillance system will help to control the current situation in the experimental cave.

3.4.10 Personnel Safety System

A PSS system will be designed in such a way that it allows the instrument team for safe operation with regards to access to the instrument through all entrances and to the operation of the positioning systems (e.g. robots) and sample environment.

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3.4.11 Instrument control

Most instrument components will require a remote control through specific electronics placed outside the shielding but connected to the components inside and to the control computers. A common protocol for communication between the instrument and any sample environment is envisaged and will be provided by ESS to facilitate plug-and-play feature. Data from the sample environments will be time-stamped and streamed to the global ESS data-stream for facilitating data reduction procedures.

3.4.12 Future upgrades options

Future upgrades can be separated into two categories. The first one consists of upgrades from the Day-one to the Full scope and can be divided into packages. One – instrument upgrades and second – SE upgrades:

Instrument upgrades will bring all missing component from Day-one scope as third PSC chopper, third and fourth FC chopper, second and third modulation chopper, missing in-plane detectors, etc. Prioritisation and draft schedule together with budget requirements are described in more detail in the proper document [8]. In the same document, detailed information can also be found for the SE upgrades from the Day-one to Full scope. The Full-scope configuration of BEER is briefly described at the end of this document

The second category of the upgrades are the upgrades beyond the Full scope. Those mainly consist in the development of new sample environments dedicated to possible new trends in material testing and production and, in an accommodation of user-designed sample environments.

3.5 Key System Interfaces

Key interfaces have to be considered carefully to embed BEER in an environment and context, which enables its optimisation and finally an efficient operation. Key interfaces are to the following systems outside the scope of BEER:

- *Target system:* This interface concerns the beam extraction guide system and its interplay with the monolith in terms of geometry, cooling and atmosphere, the utilized moderator and its choice and influence on performance and guide optics as well as the service shutter as part of the target monolith hosting a piece of the guide system and performing vital function for the operation and maintainability of BEER.
- *Bunker system:* A significant number of the most important instrument components, particularly choppers, will be placed in the shared bunker which in the BEERs instrument sector (West) extends from the monolith wall at 6 m out to 28 m with a wall thickness of 3.5 m, which implies that no choppers can be positioned between 24.5 and 28 m from the source. Interfaces with the structure, floor, columns, construction time plan, etc. have to be considered and clarified with the bunker system in the design and construction phase.
- *Conventional Facilities:* This interface and external system define parameters like the floor and ceiling heights, crane access, space for paths and infrastructure of the instrument, etc. which are all of the significant importance for the construction, operation and maintainability of the system. Placement of the material engineering laboratory about 20 m away from the BEER beam position implies that the pathway between the laboratory and the experimental cave of BEER needs to have parameters suitable for

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usage of air-pads allowing for smooth transport of heavy samples or sample environments between the instrument and the laboratory.

- *Neighbouring instruments:* There are significant physical interfaces with neighbouring instrument systems regarding space occupation which in particular close to the monolith and in the area of the instrument cave have a potential impact on the performance, availability and maintainability as well as operational access of the involved systems like choppers, etc.
- *Integrated Control System:* ICS is an important provider of key input and services for the instrument operation and in the current planning is hence vital to the instrument operation as it provides the source timing input as well as it takes up and transports key instrument data, without which the instrument becomes not operable.
- *DMSC:* The data management and software centre also provides key services and systems for the instrument in the form of control, reduction and analyses software, without which the instrument cannot be operated and exploited for its central mission. It has to be hence guaranteed that the provided software and data solutions meet the requirements of the system to function in the foreseen and useful way also for third party users and be available for Day-one.
- *Scientific Activities Division:* The SAD provides the instrument with the essential services of the user office, handling user requests and beam time proposals, hence organising the access of users required for the scientific productivity of the system according to its purpose. In addition, SAD is administrating and maintaining the common sample environment, some of which will be required to perform specific experiments on BEER and the applicability of it in the context of the BEER system has to be ensured.
- *Maintenance and Service Groups:* The integration and application of standards and corresponding solutions as well as access strategies and maintenance requirements and schedules have to be agreed with technical groups as far as possible to enable the services needed or best possible enabled through these for a high availability of the instrument system.
- *Other:* other interfaces of the system in construction (c) and operation (o) are amongst others with users (o), industry (c, o), public relations (c, o), other instruments (c, o) and in particular important for an engineering instrument with very different users and applications is an interface with data analyses specialists (c, o) which can support the best possible exploitation of the recorded data.

4. SYSTEM STAKEHOLDERS

High-level instrument stakeholders can be divided into four groups as depicted in Figure 3, the user community, industrial users, ESS, and in-kind partners.

The STAP represents the user community and the industrial users, and they formulate the science case and the purpose of the instrument. The STAP needs to be informed of the instrument design and construction progress, and it provides recommendations for the instrument team. The STAP makes a link to the high-level stakeholder – Society.

Another important group of stakeholders is the ESS facility. ESS management is responsible for delivering a top-level instrumentation to the user communities and the society. The technical groups need to ensure that the built instrument will be operational, maintainable, reliable, safe, etc.

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The in-kind partner's group of the stakeholders holds the funding organisations. In the case of the BEER instrument, there are two in-kind partners. One is the Nuclear Physics Institute of the Czech Academy of Sciences, v.v.i., representing the Czech Republic in-kind partner and the second one is the Helmholtz-Zentrum Geesthacht GmbH representing the German in-kind partner. Both partners will participate on the construction budget by 50%.

More detail description of the individual stakeholders and their role and interests within the project are listed in Table 1.

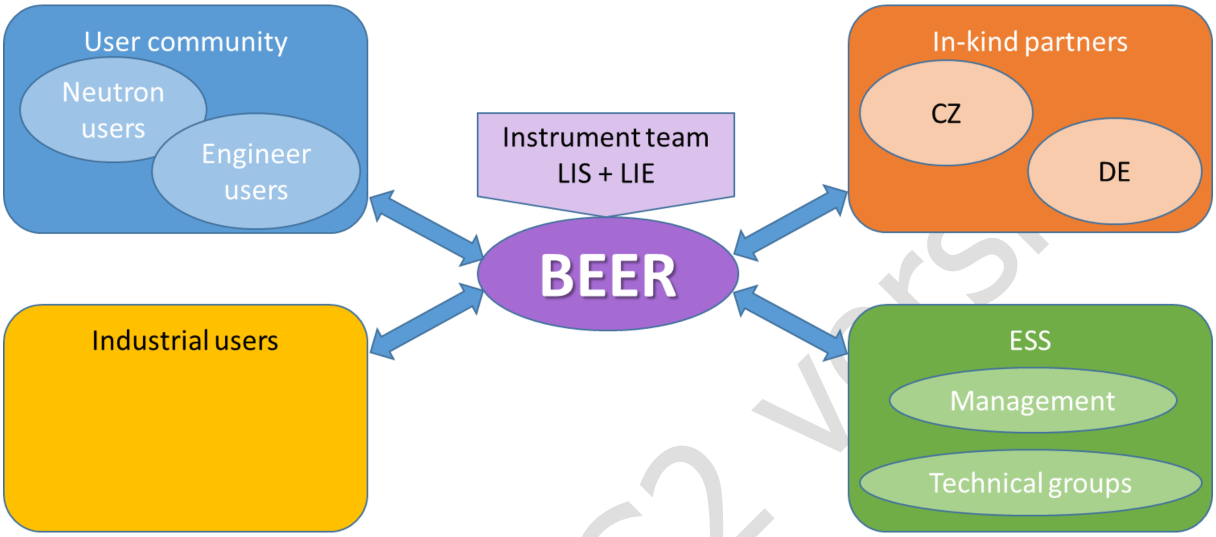

Figure 3: Basic stakeholder schematic overview

Table 1: Stakeholder list and their interests

ID	Stakeholder Group	Stakeholder	Surrogate	Interest in the project	Action by instrument team
SH-1.1	User community	Existing users of engineering instruments	STAP	Access to a world-leading instrument, perform experiments not possible elsewhere.	Regular reporting to the STAP, participation in topical conferences, dissemination of instrument progress.
SH-1.2	User community	Existing users of mechanical testing laboratories	STAP	Access to new methods to answer the scientific questions.	Participation in relevant meetings, dissemination of instrument progress.
SH-2.1	Industrial users	Potential industrial users	STAP	Access to new methods to answer the industry related questions.	Participation in relevant meetings, dissemination of instrument progress.
SH-3.1	ESS	Instrument core team	LIS (Premysl Beran, Jochen Fenske) LIE (Dirk-Jan Siemers)	Instrument delivered within budget and on schedule to hot commissioning, merit for career development.	Regular meetings and tight coordination within the core team.
SH-3.2	ESS	Instrument construction subproject	CIPE (Gabor Laszlo) CIPS (Ken Andersen)	World leading instrument delivered to hot commissioning, instrument construction project delivered on schedule and budget.	Regular meetings, timely reporting.
SH-3.3	ESS	Neutron scattering systems project	NSS PM (Shane Kennedy)	A suite of world-leading instruments delivered within schedule and budget, integration with technology development and supporting facilities.	Timely reporting when requested.

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ID	Stakeholder Group	Stakeholder	Surrogate	Interest in the project	Action by instrument team
SH-3.4	ESS	Science Directorate	DS (Andreas Schreyer)	Instrument-ready to produce scientific results early on, high scientific impact for the facility.	Timely reporting when requested.
SH-3.5	ESS	Neutron Optics Group	GL (Phillip Bentley) Group contact (Douglas Di Julio)	Good instrument performance, standardisation across instruments.	Regular meetings, ensuring coordination and integration with the rest of the instrument.
SH-3.6	ESS	Neutron Chopper Group	GL (Oliver Kirstein) Group contact (Erik Nilsson)	Good instrument performance, standardisation across instruments.	Regular meetings, ensuring coordination and integration with the rest of the instrument.
SH-3.7	ESS	Detector Group	GL (Richard Hall-Wilton)	Good instrument performance, standardisation across instruments.	Regular meetings, ensuring coordination and integration with the rest of the instrument.
SH-3.8	ESS	Motion Control and Automation	GL (Thomas Gahl)	Good instrument performance, standardisation across instruments.	Regular meetings, ensuring coordination and integration with the rest of the instrument.
SH-3.9	ESS	DMSC	Group contact (Thomas Holm Rod)	Scientifically productive instrument, data used as efficiently as possible.	Regular meetings, clearly communicated requirements.
SH-4.1	In-kind partners	In-kind contribution from the Czech Republic	Ministry of Education, Youth and Sports of the Czech Republic	Participation in the top-class facility construction. Access to world-leading instruments for the Czech community.	Regular reporting about the instrument progress.
SH-4.2	In-kind partners	In-kind contribution from Germany	BMBF	Participation in the top-class facility construction. Access to world-leading instruments for the German community.	Regular reporting about the instrument progress.

5. OPERATIONAL CONCEPTS

5.1 Operational environment

It is envisaged [9] that BEER is allocated on the beam port W2 in the experimental hall 3, building designation E01 (see Figure 4).

The instrument will be operated in a controlled environment with a temperature of 22±2°C all year round. The floor height in experimental hall 3 (E01) is about 3 meters below the target centre-line. Free height to a lifting hook of the overhead gantry crane is maximum 10 meters with maximum load of 10 tons[1]. Floor loading in the experimental hall 3 must not exceed 20 tonne/m[2]. Floor stability in the hall is specified to be maximum 3 mm w.r.t. elastic movement and another maximum 3 mm due to creep/deformation.

Utilities and media are brought to the instrument from the gallery. Media include N_2, instrument grade compressed air, cooling water low. Utilities include office IT, office comms, power, MPS, PSS, DMSC, and ICS. For a detailed and updated listing of requirements and specifications related to operational environment see the System Requirements Document. Details for e.g. maintaining the stable temperature in the experimental hall are still in development, but one

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[1] According to ESS-0052338

suggested solution could be to place ventilation hoods directly above instrument equipment generating the most heat.

The ESS facility has five different operating modes [10]: Shutdown, Studies, Studies on Target, Startup, and Production. These modes have various impacts on instrument operations. Pure experimental work can only be conducted during the Production mode. Access to instrument equipment for maintenance, calibration, cold commissioning is mainly done during the shutdown, studies and studies on Target – naturally after due safety assessment. During start-up, instrument operations are limited to alignment, commissioning and calibration runs.

When ESS enters into a steady-state operation phase, the following principal schedule is currently expected to apply:

- 200 days/year of neutron Production for the ESS users after 2026,
- Proton beams will be on target for ~225 days/year,
- Two long Shutdowns, one in winter (~6 weeks) and the other in summer (~10 weeks) followed by Studies and Studies on Target periods,
- 3 Optional Studies Days every second week to avoid long downtime of instruments due to failures of activated components, followed by 2 days for Studies and Studies on Target,
- A series of Studies days to allow for fine-tuning of accelerator and target systems.

One goal of ESS is to ensure that at least 90% of the users receive a neutron beam allowing them to execute the full scope of their experiments. This is in accordance with the availability and reliability assessments declared in [11][12].

The BEER instrument is foreseen to be managed and operated by a team of 2-3 scientists and one engineer. ESS will be manned 24 hours/day, seven days a week, not all categories, but this manning will allow for flexibility for users when conducting experiments and making preparations or analysing results.

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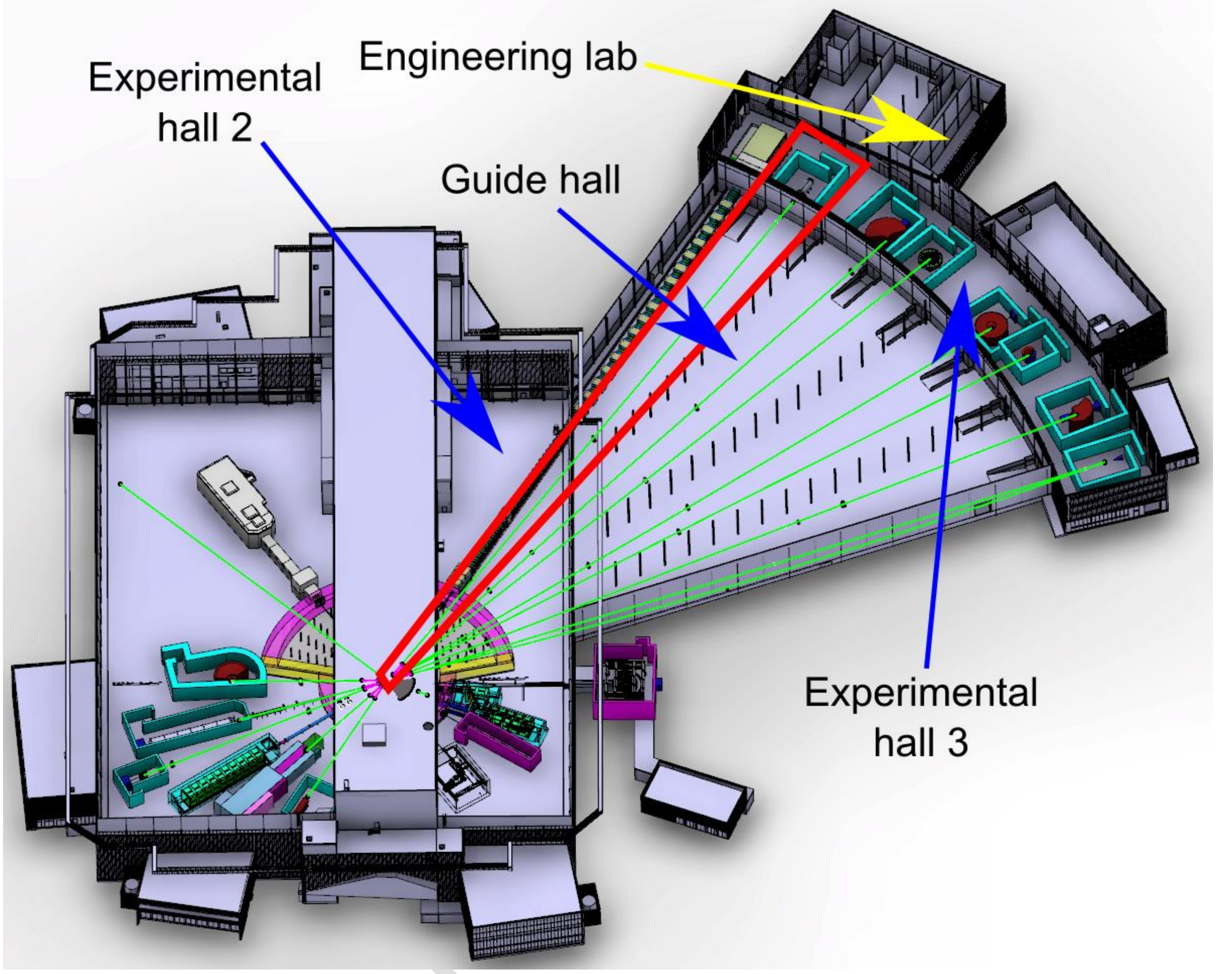

Figure 4: The allocated beam port (red rectangle) for the BEER instrument according to [9]. Main buildings where neutron guides will path are also indicated.

5.2 Users and user operation scenarios

A neutron scattering instrument is a user facility, which means that the experiments are conducted by scientists (academic or industrial) from all over the world. The BEER instrument team provides scientific and technical support and advice to these experiments, but the users perform the actual experiment. The beamtime for user experiments is allocated through a peer-review process based on scientific merit and feasibility. Proprietary access for industry partners is also envisaged.

The typical users of the BEER instrument will be scientists or industry partners studying phase transformations, mechanical properties of engineering samples as a function of material status, internal strain and texture parameters of complex shape samples and other similar topics from the materials engineering research. The level of user experience varies from one-time users to regularly experienced users of neutron scattering techniques. BEER has envisaged to accommodate dedicated sample environment, which is often used in material testing laboratories, adapted in such a way that it can be installed on a neutron diffraction beamline. This would potentially attract users from engineering laboratories, who are familiar with these types of sample environment devices (like deformation rigs, dilatometers, Gleeble®, etc.) but have limited or no experience with neutrons. The user team would typically consist of 1-4

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scientists (Ph.D. level or doctoral students) who perform the experiment within the allocated beamtime. They bring their samples with them, ship them beforehand, prepare them using the ESS supporting facilities or dedicated BEER engineering laboratory, or bring samples along with their own sample environment equipment. The team is expected to operate the instrument 24 h per day, even though they may not be continuously present at the instrument.

A remote status check of experiment flow is also envisaged to monitor long sequences of measurements and to catch sight of possible problems with sample environments or the instrument itself.

The users will process the data using specialised BEER data reduction and visualisation software at least up to a point where a data analysis software can further process it. Depending on the mode of operation, the reduced data can have different forms. For simple diffraction mode (as strain scanning, simple *in-situ* deformation experiments), the reduced data consist typically of an indexed list of fitted parameters of individually scaled reflections as a function of sample environment status.

5.3 Operational scenarios

BEER is designed as a very versatile instrument able to accommodate different sample environments and use different techniques (diffraction/imaging) which require adequate adjustment systems. For the manipulation of the neutron beam to the experimental needs, a complex chopper system and advanced focusing guides are used. To make the best use of the long ESS pulse, a novel technique, called pulse modulation, was introduced. It enables measurements with high resolution and high intensity for high symmetry materials. A description of this technique as well as different operation modes are briefly described in the following chapters.

5.3.1 Modulation technique

The pulse modulation technique works as follows: Looking at the time distance diagram from the detector to the source one sees that, for a given detection time, the source pulse with a length of 2.86 ms creates at the first modulation chopper position (about 9 m from source) a virtual source with a pulse length of 2.86 ms × 150 m / 159 m = 2.70 ms – this time interval is to be extended a bit due to the afterglow of the source. The modulation chopper subdivides this long virtual source pulse into a pulse train with a pulse to pulse distance δt_{ptp} depending on the frequency and the slit distances of the first modulation chopper disc, which results in the consecutive, in total M_d =2.70 ms / δt_{ptp}, pulses, which arrive at the detector well distinguished in wavelength. M_d is called a *multiplexing degree*. At the highest frequency of 280 Hz and 16 chopper windows, up to 12 such sub-pulses are formed during the 2.70 ms period. At a lower frequency, the pulse is less split (e.g. M_d = 3.5 for f = 70 Hz). Note that M_d is not necessarily an integer. The pulse splitting results in multiplexing of Bragg reflections (for more information see [3]), which can be used to reconstruct a single Bragg peak with M_d times higher intensity and high resolution.

This operation mode is a huge advantage, e.g. for speeding up residual strain mapping or, under suitable conditions, for increasing the time resolution of in-situ experiments. This advantage is limited to high symmetry materials where the trains of sub-pulses from different lattice planes do not overlap. A similar problem of sub-peaks overlap may arise due to the intrinsic peak broadening. Therefore, an experiment simulation will be needed to adjust the multiplication factor M_d (by choosing another frequency or another chopper disk) to ensure sufficient sub-peak separation. This method also requires dedicated data processing software

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allowing for selection and fitting of non-overlapping data regions in the 2D space of TOF and scattering angle.

5.3.2 Operation modes

Operation modes can be classified according to different criteria: resolution, experimental method, sample environment. The basic classifications are described below.

Intensity and resolution

BEER can be operated in a significant number of modes providing different intensity/resolution conditions according to the experimental needs. Typical modes classified according to the trade-off between *intensity* and *resolution* (IR modes) are listed in Table 2.

Table 2: List of basic instrument modes described as trade between resolution and intensity.

IR modes	PSC[*]	modulation	diverg. Slit	focusing guide	Δλ/λ [%]
medium resolution (MR)	1+2[***]	-	40 x 80	no[**]	0.3
high resolution (HR)	1+2[***]	-	15 x 80	no	0.1
modulation high resolution (MHR)	-	280 Hz	10 x 80	no	0.07
modulation low resolution (MLR)	-	70 Hz	40 x 80	no[**]	0.27

(*) Pairs of Pulse Shaping Chopper in operation
(**) vertical focusing is possible for the detectors near $2\theta=90°$
(***) Pulse shaping chopper 2 is translating along the beam

The basic wavelength bandwidth available at the sample position during one source period is 1.7 Å (*single frame*). Using the pulse suppression technique (for more information see [3]), it is possible to extend the wavelength range by selecting one continuous frame of 3.4 Å (*a double frame*). The double frame mode can be used only with the modulation technique due to the frame overlap problem. The centre of the wavelength range can be selected as needed by proper phase adjustment.

Experimental method

Operation modes classified according to the used methods can be summarised as follows:

- Diffraction – only diffraction data are required, resolution, mean neutron wavelength and divergence slits are adjusted according to the necessary d-range and $\Delta d/d$ resolution. Applicable IR modes: MR, HR, modulation mode (anything between MHR and MLR). Wavelength selection: single frame or any of the pulse suppression modes. Experiment type (see Chapter 2): I, II, III, and IV.
- Diffraction and imaging – truly simultaneous measurement of diffraction and imaging is probably not possible due to different beam requirements, but the instrument will allow for rapid switching between the diffraction and imaging setups by slit adjustments. Bragg edge imaging requires only moderate TOF resolution and can thus be performed in any of the pulse shaping modes (MR, HR). Imaging is considered as an auxiliary method e.g. for monitoring homogeneity of phase transformations during in-situ tests, sample positioning or 2D mapping of strains and textures in flat samples.

Sample environment

Further classification of operation modes can be done by the sample environment used, for example:

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- Thermo-mechanical experiment using a deformation rig
- Heating experiment with a furnace
- Sample scanning experiment using a robotic arm or hexapod
- In-operando experiments using specialised environment, e.g. for forging or welding

A special mode with active sample environment feedback is also envisaged. In this mode, the procedure on the sample environment is modified by data derived from a simple real-time data analysis. A quenching procedure can be used as an example. The sample is cooled down slightly below the transformation temperature. The phase transformation takes place with a dwell time at this temperature. Then the sample quickly cooled down. The dwell time and the transformation temperature may be unknown and have to be determined (the purpose of the experiment) in such a way that the final material has a predefined phase composition. The in-situ fast data analysis can evaluate the phase fractions and actively control the dwell time or temperature depending on pre-set criteria (like the phase fraction value).

Due to this large variety of possible operation modes, a complex description is needed to underline all aspect of instrument setup and sample environment used.

5.3.3 Step-by-step experiment

This section provides a step-by-step description of all stages of an experiment on BEER. Numbers in the brackets refer to the experiment types to which individual steps are applicable (see Chapter 2). If nothing is mentioned then, the step applies to all experiments.

A. Instrument preparation (cave: open, beam: off, staff: scientist, engineer)
  - installation of SE hardware (I, III, IV)
  - installation of a robot or another positioning system (hexapod, cybaman, etc.) (II, III)
  - optical alignment of SE on the sample table (I, III, IV)
  - setting and connecting of all auxiliary equipment (cooling water, heating system, different SE sensors, etc.) (I, III, IV)
  - checking of all functionalities using remote control

B. Sample preparation (cave: open, beam: off, staff: user, scientist,)
  - sample shape and dimension is needed to be discussed in advance or in special cases it can be adjusted in general or engineering workshop (I, II, III)
  - placement of the sample into SE, this can be done in some cases already in advance outside the experimental cave in engineering laboratory (I, III)
  - optical alignment of the sample within SE (I, III)
  - in the case of big samples, setup on the universal platform within the engineering laboratory and transport using air-pads to the experimental cave (II, III)
  - 3D scan of the sample and transfer of its coordinates to the sample positioning system (II, III)
  - alignment of the sample with respect to the beam centre (II, III, IV)

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- if the multiplexing technique will be used, run of the virtual experiment is needed to properly set-up the multiplexing degree(see chapter 5.3.1)

C. Sample environment preparation (cave: open, beam: off)

- design and test of SE procedure in engineering laboratory (I, III)
- programming of SE procedure (I, III)
- verification of all sensors connections and signal readout (I, III, IV)
- programming of the sample scanning pathway and rotation (II)
- programming of the sample movement and/or rotation procedure (III)

D. Hot setup (cave: closed, shutter: open, beam: on)

- checking the alignment of the sample by a neutron camera
- remote sample re-alignment if necessary
- checking of the detector signal and position for all used ones (diffraction or imaging detectors), radial collimators alignment (for in-plane and off-plane detectors if needed), adjustment if necessary
- adjustment of the chopper system based on the experimental needs
- adjustment of the apertures and focusing optic
- checking of the beam characteristics on controlling beam monitors

E. Measurement (cave: closed, beam: on)

- the sample is exposed to the beam
- scattering data are collected in event mode
- procedure on SE is launched (I, III)
- the script of the sample movement/scanning pathway is launched (II, III)
- live-view of the measuring data is available
- if active feedback is active then fast data analysis taking place and SE procedure is adjusted based on its results (I, III)
- long SE procedures will be run for a significant time without external control
- exposure and data collection are interrupted in most cases when the source has downtimes but resumes when the source reaches a threshold neutron production again, if necessary those interruptions can be omitted and SE procedure will continue event during the source downtime

F. Sample exchange or removal (cave: open, beam: off)

- the sample is scanned for activation
- potential waiting time than the sample cools down under threshold activation
- sample removal, by hand or with remote tools (activation) (I, II, III)
- removal of whole SE hardware (IV)
- sample storage (activated/non-activated) (I, II, III)

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- installation of the new sample if needed and repeat the procedure from point B. (I, II, III)

G. Additional sample characterization

- further instant examination of the samples after the in-situ procedure using an optical microscope (cracks characterization, surface conditions, etc.) in the engineering laboratory (I, II, III)

H. Data analysis

- data reduction is done as soon as possible; proper time stamping of the SE outputs is needed to attribute each neutron event to SE status
- quick visualization of data as a function of selected sample environment status facilitate a discussion for the next sample planning
- data format need to have a form acceptable by analysing software (diffraction or imaging data), it is basically 2D histogram of normalized intensities in 2θ vs TOF (wavelength), or 1D histograms on the d-spacing scale in the case of diffraction data.
- data analysis is mainly done at user home laboratory or in collaboration with the instrument scientist together with DMSC, some preliminary data analysis can be done during the allocated beamtime using the instrument hutch resources
- online access to the data reduction software by the user help to overcome the problems during hurry-up data reduction within the allocated beamtime

5.4 Maintenance Concepts

5.4.1 Levels of maintenance

Within ESS there are three identified levels of maintenance which are described in [10]:

1. *Organizational maintenance:* maintenance performed on site where the component is normally being operated,
2. *Intermediate maintenance:* maintenance performed on site at a dedicated workshop,
3. *Supplier maintenance:* maintenance performed off site at the supplier premises.

The suppliers also include scientific partners as e.g. In-Kind partners.

5.4.2 Maintenance categories

Maintenance can be divided into two categories: *Corrective* and *Preventive*. By utilising condition based monitoring, taking into account the overall ESS operational schedule, preventive maintenance on instruments is aimed to be conducted during the planned facility shutdown periods unless instrument reliability and availability are sacrificed. This will minimise disruption to a user operation.

Preventive maintenance is part of scheduled maintenance which also includes maintenance work to be conducted on equipment where condition based monitoring cannot be achieved. Performed instrument reliability analysis, part of RAMI work, aims to ascertain that preventive maintenance on this type of equipment/components could be limited to periods of scheduled shutdown of the facility. Maintenance and monitoring requirements of critical components will be taken into account in design and procurement of equipment from the beginning.

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Corrective maintenance will mainly apply when an event happens to force the maintenance to be done unscheduled. This occurs when either a component has a failure, or an issue that requires immediate action during user operation has been detected. The instrument will have to stop user operations for the duration of repairs or maintenance.

Another key categorisation of maintenance is the distinction regarding access requirements and limitations. Components can hence be categorised into easy maintenance access, limited maintenance access, and difficult maintenance access devices. In the first category, all devices and components can be placed in areas which are located outside the radiation shield of the instrument, including such devices placed in the experimental cave. These devices can be serviced anytime when required, though downtimes are used for preventive maintenance in order not to interfere with the scientific utilisation of the instrument. In the second category are the limited number of hardware components installed in instrument shielding downstream of the safety shutter system, i.e. between the bunker shield (at 28 m) or wavelength selection chopper (at 80 m) on one side and the experimental cave on the other side. These components shall be accessible during source operation in case of required corrective maintenance. In the third category are components installed upstream from the safety shutter and within the bunker area where access currently appears to be possible only during source downtimes and through remote handling. Access to components within the last two categories requires removal of shielding with the corresponding implications of crane use, space requirement and scheduling and additionally, might also involve a required cool down time of components due to activation, which increases times needed for the maintenance.

Another category of practically no access components as the extraction system in the monolith could be defined, which are almost non-accessible, as access requires removal of significant parts of the instrument and its neighbours. Hence, no moving parts and components requiring maintenance can be placed there and the design of the components installed there has to be especially robust.

5.4.3 Maintenance philosophy

BEER's maintenance philosophy is in line with the approach of the facility to utilise conditions based on preventive maintenance as much as possible. In order to minimise required resources and potential instrument downtimes, an application of the facility standards is in the focus of an instrument design. So-called "failure mode operations" are also planned, where the instrument can be operated in a usable mode even in the case of a component failure which does not permit immediate maintenance. However, performance and in particular cost against a usability within a very limited instrument budget are major constraints and hence balanced cost-benefit solutions are indispensable.

The most critical components with regards to the maintenance can be easily identified: they include all moving parts within the bunker and instrument shield upstream from the sample. For BEER, those are the exchangeable focusing guides, all types of choppers (PSCs, FCs, and MCs) and the safety shutter. The following philosophies apply to those in the BEER design.

Exchangeable focusing guides:

- Each stage can be removed separately from the lift mechanism used for their exchange.
- If the lift has to be removed, a holder for a single stage should be available for replacement; this ensures the instrument availability.
- Removal of the system shall not affect the rest of the guide system.

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- Each stage should have its independent vacuum housing unless engineering reality requires a common housing.
- Vertical removal of the entire lift and remote handling are foreseen.

Chopper systems:

- Choppers are accessible and removable vertically from the top, and when required by remote handling. However, up to date, there is no information available on expected activation and radiation situation within the bunker. The bunker concept is yet to be clarified, especially on the amount and level of activated material (e.g. T0 choppers and heavy shutters) and shielding inside the bunker. Better knowledge of the situation to be expected is essential to plan resources efficiently and under correct assumptions.
- Choppers are removable out of the bunker (PSCs, MCs, and FC1) or shielding (FC2). This may affect the guide system after the monolith if the guide segments are integrated with the vacuum housing of the choppers. This implies state of the art split housing approach for choppers which are connected to the guide vacuum system, which is a design driver on performance to keep guide interruptions as small as possible.
- Chopper discs can be turned to an open position (PSCs and MCs). This is necessary for BEER as simulations clearly demonstrate that some of the modes that BEER enables stay functional in the case MC or PSC choppers need maintenance due to failure and cannot be removed out of the bunker immediately (proton beam on target has to be off to access the bunker).
- Chopper solutions with minimum maintenance requirement (magnetic bearings) are preferred where affordable, final choice requires cost-benefit analyses. Failure mode operation enables maintenance with a certain frequency.

Safety shutter:

- The safety shutter has to be designed as a fail-safe. Hence, the design has to foresee shutter operation even if the primary system fails.
- Removal of the shutter disables any instrument function. Hence, the component has to be designed as maintenance-free as possible.
- Removal is vertical, with remote handling as required and with no impact on neighbouring components.

Sample environment:

- The design of the sample exposure system has to be designed in a way allowing for installation of standard sample environments from the ESS pool. This ensures fast and easy replacement for similar equipment in the case of failure.

Detectors:

- The detector system is subdivided into exchangeable building blocks. The neutron sensitive part of the read-out electronics is planned, as far as compatible with the application, to consist of identically constructed components. In the case of failure, the broken component could be replaced temporarily by locally available parts from unused detectors.

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- For the active protection of the detectors, an overexposure monitoring system is planned which can close available shutters or ramp down the HV at the concerned detector.
- It is foreseen to install into the detector system a remote control and monitoring system to read the status of the detector via a secure internet protocol. In this way, skilled and experienced engineers can quickly warn the instrument scientist before costly damages accrue and check long term drifts and development of key parameters.

The guide system should not require maintenance, but in the case of failure a partial removal follows similar principles as for the choppers. Some choppers may need to be removed as well. Realignment requirements for the guide are to be considered in the general design of the system, and the guide design shall be robust against misalignment as much as possible with respect to cost and performance. Provisions for regular neutron flux measurements at suitable points (bunker exit, safety shutter, etc.) should be made to signal guide degradation or misalignment.

All other components are accessible, should be quickly replaceable (standards) or allow failure mode operation, partly through replacement by alternative components (e.g. different detector to be used). Regular maintenance and check according to suppliers' recommendations shall prevent failure.

6. CONSEQUENCES OF THE CONCEPTS

6.1 General design considerations

General design considerations concern all functional and non-functional requirements and are/will be documented in detail in the corresponding documentation.

6.1.1 Upgrade options

Identified upgrade options shall be considered and be catered for as much as possible in the design solutions, see Chapter 3.4.12.

6.1.2 Robust design

The current preliminary design can be regarded as robust with respect to the scientific and technical aspects raised. This is supported by the flexibility and various available failure modes of the instrument, which allow for efficient operation in nearly all cases of single component failure. However, careful provisions have to be made in particular also during final design and especially the performance, and respective corresponding issues of the extraction guide and the guide curvature have to be considered carefully. The final design of the guide including its alignment and support as well as choices still to be made on details of choppers and their support will be of significant importance.

The failure modes are particularly considered in the case of a chopper failure. The instrument is designed to be able to operate in another mode to allow usage of the full user beamtime.

However, robustness has also to be considered with respect to viable systems that BEER is connected to and relying on. This concerns particularly the ICS and data streaming functions coupled with it. In order to guarantee best possible availability, it is foreseen that BEER is able to operate in a stand-alone mode in case of difficulties of the ICS and data streaming systems. The only precondition required for all instrument modes is receiving a trigger signal from the source pulses, which BEER hence demands to get supplied with through a hardware solution.

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A control of the opening position/phase of the chopper disc which defines wavelength resolution by a simple photoelectric guard allows for reliable estimation of t_0 (needed for determination of the neutron TOF) and control of phase stability of the chopper system. With such a system, the required resolution in TOF and therefore $\Delta\lambda/\lambda$ as well as phase stability of choppers can be monitored and ensured.

All choppers can usually, just like other motion control be addressed locally either through internal hardware connection or in the worst case by directly approaching the specific electronics or controls in the case of difficulties with the ICS. The sample environment solution considered the local storage of tagged data for possible re-alignment with scattering data. Detector solutions should consider local data storage capability (for limited volumes and time) and hence allow for stand-alone operation of the instrument for considerable downtimes of centralised capacities.

Robustness is also considered with respect to the temporary source failure. It is important for material scientists to continue thermomechanical experiments during a source failure. The system allows such regime and stores all SE data locally during such interruption.

The failure of the SE, in particular for BEER, will have consequences for beam-time usage. In such a case, the free beam time can be assigned to a pending long-term experiment, at which the precise timing of neutron measurement is not an issue. This maximises the beam usage.

Better knowledge of the operational environment and interfaces like with the target, but in particular, also the conditions during access in the bunker are key boundary conditions to enable optimum choices and design.

6.2 Training of personnel

The instrument scientists have to maintain a research profile and dedicate time to the scientific research in order to understand the needs of the existing and future user community. Post-docs working at the instrument can support the operation by engaging in methodological developments and participating in user support.

The technical support of the instrument operation would include mechanical, electrical, software and other speciality engineer and technician personnel, who could be part of the instrument team or in specialised technical groups.

A dedicated technical and engineering support will be needed for the SE. A huge variety of specialised SE is needed for successful operation of the BEER instrument. The dedicated SE engineer should be a part of the instrument team.

The users arriving at the instrument to perform experiments will be supported by a local contact such as one of the instrument scientists. The more experienced users should be able to operate the instrument independently after a short (< 1h) introduction by the BEER instrument team and the less experienced users who would require more support would be expected to establish a collaboration with BEER scientists.

7. FULL SCOPE INSTRUMENT

The Day-one configuration of BEER fulfils the high-level scientific requirements defined at the beginning of the document. Some of them, however, are restricted due to the reduced scope, e.g. the capabilities to measure textures or to combine SANS and diffraction measurements for in situ studies. The full advantage of BEER compared to existing engineering

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diffractometers will only become available in its Full-scope configuration. Therefore it is important to discuss also this configuration in respect of the Concept of Operation.

While the previous chapters reflect the Day-one configuration of BEER agreed on at the scope setting meeting [2], changes to some sections occur when BEER is upgraded to its Full- scope configuration during staging. This affects not only the System Overview when adding additional components like detectors or choppers but also the Scientific Requirements and Operation Scenarios when new methods and instrument abilities become available.

These changes will be discussed in the following text structured in the same way as for the whole ConOps document.

7.1 Full scope scientific requirements

In the Full-scope the requirements which have limitations in the Day-one configuration (see section 2.2) will be required in full. Requirements 6. and 10. will have different limits:

6. The detector coverage together with the available wavelength bandwidth shall be optimized for a sufficient d-range for common engineering materials which is identified as 0.7 - 9 Å. (I, II, III, IV)

10. BEER shall allow d-resolution (Δd/d) to be optimized for the experiment (0.1% < Δd/d < 0.6 %) by trading intensity for resolution. (I, II, III, IV)

And there are foreseen more scientific requirement in the Full-scope which are not presented in the Day-one:

- BEER should allow for collecting SANS data simultaneously with diffraction. (I, III, IV)
- The detector coverage shall allow the measurement of an almost complete intensity pole figure for texture analysis by rotation of the sample around one sample axis. (III)
- The detector coverage shall allow monitoring of partial texture evolution without sample rotation during an in-situ experiment when the sample itself or sample environment does not allow the rotation because of its size and/or technical construction (cryostats, ovens, etc.). (I, III)

7.2 System Overview

7.2.1 Sample exposure systems

Additionally to the sample exposure systems discussed in section 3.4.7 a heavy load table for z-movement will be installed under the rotation table. Both systems together will serve as the main positioning system for other equipment.

An optical tracking system for increasing the precision of the positioning system is envisaged in the Full scope of BEER. The final solution for this system is not yet set. It needs to take into account the complexity of the sample environment used and the limited space of the instrument cave.

7.2.2 Detectors

Additional to the Day-one detector configuration described in section 3.4.8, the following detectors are foreseen in the Full scope of BEER: Two additional in-plane detectors at 50°and 130° with the surface of 1x1 m^2 at distance of 2 m. A smaller detector at a shorter distance (~1.5 m) and medium resolution (~5x5 mm^2) will be placed on one side of the incident beam for backscattering measurements.

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A 1x1 m^2 detector for SANS measurements (displaced from the direct beam to increase the dynamic Q-range) will be placed in a vacuum tank at up to 6.5 m behind the sample. This distance is determined by the distance of the divergence slit in front of the sample, which will be used for both diffraction and SANS.

An arc with detectors filling the space between the 90° detector and zenith improves the detection coverage for texture and strain analysis. It is to be mounted on a construction built above the sample stage, with the possibility to free the space for large sample environment when needed. A shorter distance (~1.2 m) and smaller detection area (3 segments, 0.5x0.5 m^2 each) should be sufficient for this purpose.

7.3 Users and user operation scenarios

The full-scope configuration of BEER includes additional to the diffraction and imaging methods also optional SANS measurements. Therefore different operation scenarios are possible. For very advanced modes, the diffraction data represented as a 2D pattern of normalized intensities in space of diffraction angle vs. TOF (from all applicable detectors) are combined with the sample environment data as well as SANS data represented by an array (1 or 2 dimensional) of values of macroscopic differential scattering cross sections (normalized intensities) as a function of the scattering vector (Q).

7.3.1 Operation modes

The full scope configuration includes a third PSC disc which enables the high flux mode of BEER. Therefore table 2 in section 5.3.2 can be extended as follows:

Table 3: List of basic instrument modes described as trade between resolution and intensity.

IR modes	PSC	modulation	diverg. Slit	focusing guide	Δλ/λ [%]
high flux (HF)	1+3	-	40 x 80	yes	0.6

The frame definition choppers FC1 and FC2 will be upgraded in the Full scope to double disc systems allowing beneath the double frame mode to select two 1.7 Å frames separated by a 1.7 Å gap (*alternating frames*). While the double frame mode can be used only with the modulation technique due to the frame overlap problem the alternating frame mode can also be used with the pulse shaping technique. Both techniques permit to employ simultaneously thermal and cold neutrons, e.g. for combined diffraction and SANS measurements.

The additional SANS option allows another experimental method:

- Diffraction and SANS – simultaneous measurement of diffraction and SANS data in the Full scope configuration of BEER. The resolution, mean neutron wavelength and divergence slits are selected according to the required d-range and resolution for diffraction, as well as the size of expected microstructure to be monitored by SANS. Applicable IR modes: HF, MR, HR, multiplexing mode (anything between MHR and MLR), but the reduction of beam divergence may be needed for sufficient SANS resolution. Wavelength selection: alternating frames or double frame (only with pulse modulation). Experiment type (see Chapter 2): I and IV.

7.3.2 Step-by-step experiment

The full-scope configuration of BEER enables SANS, therefore, step E. (Measurement (cave: closed, beam: on) of the step-by-step experiment has to be extended in case of SANS measurements by:

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- perform calibration measurements (empty beam, empty SE, standard, etc.) when SANS option is used (I, III)

and step H. (Data analysis) by

- in the case of SANS data are represented in the form of an array of scattering cross-section values, either as a 2D map, S(Qx,Qy), or azimuthally averaged 1D data, S(|**Q**|), or slit-smeared (vertically integrated) 1D data, S(Qx).

8. GLOSSARY

Abbreviation	Explanation of abbreviation
BEER	Beamline for European materials Engineering Research
BMBF	Bundesministerium für Bildung und Forschung
CDR	Critical Design Review
CIPE	Chief Instrument Project Engineer
CIPS	Chief Instrument Project Scientist
ConOps	Concept of Operation Description
DLS	Direct Line of Sight
DMSC	Data Management and Software Centre
ESS	European Spallation Source
FC	Frame selection Chopper
FWHM	Full Width in Half Maximum
GL	Group Leader
HF	High Flux
HR	High Resolution
ICS	Integrated Control System
IRR	Installation Readiness Review
LIE	Leading Instrument Engineer
LIS	Leading Instrument Scientist
MC	Modulation Chopper
MHR	Modulation High Resolution
MLR	Modulation Low Resolution
MR	Medium Resolution
NSS	Neutron Scattering Systems
ODIN	Optical and Diffraction Imaging with Neutrons instrument
ORR	Operation Readiness Review
PCS	Pulse Chapping Chopper

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Abbreviation	Explanation of abbreviation
PDR	Preliminary Design Review
PSS	Personal Safety System
Q	Scattering Vector
RAMI	Reliability, Availability, Maintainability, and Inspectability
S/B	Signal to Background ration
SAC	Scientific Advisory Council
SAD	Scientific Activities Division
SANS	Small Angle Neutron Scattering
SAR	Safety System Acceptance Review
SE	Sample Environment
STAP	Scientific and Technical Advisory Panel
TG	Tollgate
TOF	Time Of Flight

9. REFERENCES

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DOCUMENT REVISION HISTORY

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0.5	New Document	2015-05-14
0.6	Updated template based on ODIN&NMX ConOps	2016-05-10
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