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Scope Setting Report Instrument: Engineering Diffractometer BEER

SUMMARY

This document describes three baseline options for the scope of the diffractometer BEER and consequences of associated cost saving strategies on the instrument performance and science drivers as they are envisaged in the instrument proposal [1].

The first option represents an attempt to reduce the instrument scope under the limit of the cost category B (12M€) assigned to BEER while preserving a maximum of its performance. The second option allows delivering a world class engineering diffractometer on day one, with the possibility of a subsequent upgrade to the full scope described as option three. This full scope then meets all performance and scientific requirements of the originally proposed instrument [1].

It is concluded that BEER cannot be delivered within the cost category B without sever downgrading of both performance characteristics and research opportunities. Moreover, such an instrument would not allow for a future upgrade without overall reconstruction. On the other hand, the option two is a viable plan for the delivery of a world leading engineering diffractometer while reducing the initial construction costs significantly.

TABLE OF CONTENT

PAGE

1. OVERVIEW

1.1. Science Case

The grand challenges of modern society originate in the priorities of a sustainable development of modern technologies and our interest in the improvement of everyday life including e.g. computers, batteries, food, medicine, transportation, and energy. Technological progress relies heavily on the improvement of materials. The development of materials with high performance and tailored functionality is based on fundamental understanding of the relation between the microstructure and properties of material. This also requires the development of new and improved experimental tools for precise and reliable characterization of materials.

Progress in development, fabrication, optimisation, and degradation monitoring of modern engineering materials is essential for the production of more efficient, more environmentally friendly and more durable engineering components. To achieve such ambitious goals, employment of science-based approaches towards material design and development as well as the adoption of new methods for production, thermomechanical processing, testing and characterization of materials is required.

Neutron diffraction has become a well-established experimental method of engineering sciences for microstructure characterization of materials for industrial applications. The conventional use of neutron diffraction lies in the field of phase, residual stress and texture analysis, as well as defect and nanostructure analysis; however, the complexity of materials of interest as well as the experimental methods have changed significantly in recent years, with in-situ and in-operando experiments becoming more important. The reason is that not only the microstructure but also the processing techniques for the production of modern materials have become increasingly complex, and further progress can often only be made when the time-dependent processes are studied under production-like conditions in real time. Particularly for material engineering research, it will be extremely helpful to replicate real fabrication, processing and in-operando conditions in neutron beams. It will move analytical processing and performance research from post-mortem analysis to yet unparalleled in-situ or in-operando analysis. Such research will lead to breakthroughs in the optimisation of various engineering materials processing, e.g. development of advanced methods of joining such as friction stir welding or improvements of industrial processing such as casting, hot rolling, forging and annealing. Therefore academic as well as industrial users will benefit from new in-situ and in-operando neutron diffraction experiments.

The unique concept of BEER was developed to offer these possibilities. The full scope instrument is based on a significant improvement in data acquisition times compared to current materials engineering flagship instruments, a flexible detector coverage, additional small-angle scattering (SANS) and imaging options and complex sample environments. The concept is mainly driven by:

(I) enabling time-resolved in-situ and in-operando investigations of structure and microstructure of materials during processing and/or exposure to simulated service environments and conditions,

(II) adopting state-of-the-art technologies for efficient and precise characterization of residual stresses, crystallographic textures and phase compositions in structural materials.

Thus, new opportunities will be offered to material engineers for studying the evolution of micro and nanostructures, phase transformations, textures and internal stresses at industrially relevant temperatures, strain rates and complex loading conditions. This will help to investigate and develop thermomechanical processing procedures as well as to study fatigue mechanisms under service conditions.

Furthermore, BEER will allow for long-term experiments studying slow engineering processes, e.g. fatigue, corrosion, creep. Those slow processes will be checked on the beam only a few times per month or year. Most of the time the experiment will be running ex-situ in the dedicated engineering laboratory or in the preparatory lab and will be transported from and to the instrument cave using a universal transport platform. A sensitivity of some of those experiments to the change of external conditions is crucial which implies the necessity of close connection between the elevated experimental cave and the laboratories on the ground floor with a smooth passage.

1.2. Requirements

The top level requirements for BEER [2] define the target scope for the instrument construction project. They have been formulated to capture the key aspects of the instrument proposal science case and are:

- 1. BEER shall allow the measurement of nuclear and/or magnetic structural data.
- 2. BEER shall allow the collection of scattering data in-situ and in-operando using a variety of sample environments.
- 3. BEER shall allow the scanning of residual strains within complex shape samples with high throughput.
- 4. BEER shall allow the measurement of microstructures (lattice strain, micro-strain, texture, etc.).
- 5. BEER shall allow the long-term experiments.
- 6. The detector coverage together with the available wavelength bandwidth shall allow access to a sufficient d-range for common engineering materials which is identified as $0.6 - 9$ Å.
- 7. 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.
- 8. 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.).
- 9. The instrument shall allow measurements of two strain components at once.
- 10. The experiment control shall allow users to choose a continuation (besides standard pause procedure) of the material test experiment after an interruption of the neutron beam due to a temporary source failure.
- 11. The experiment control shall allow in-situ experiments driven by the sample environment with an active feedback.
- 12. BEER shall allow the gauge volume to be adjusted for the experiment down to about 1 $mm³$.
- 13. BEER shall allow data to be collected to d_{min} of about 0.7 Å for detectors at 90°.
- 14. BEER shall allow d-resolution (Δd/d) to be optimized for the experiment (0.1% < Δd/d < 0.8 %) by trading intensity for resolution.
- 15. BEER shall provide sufficient space for large sample environments.
- 16. BEER shall allow the placement of heavy samples and/or sample environment with a total weight up to 3 tonnes.
- 17. BEER should allow for collecting SANS data simultaneously with diffraction.
- 18. BEER should allow for direct imaging over a 40x40mm² field of view with energy resolution sufficient for Bragg edge contrast enhancement.

1.3. Configuration options

Three configuration options are presented:

- 1. A configuration that is within the cost category B (12M ϵ). The aim was to meet the cost category for the construction phase. Cost: 12 M€
- 2. A configuration that manages to meet the most important scientific requirements at reasonable performance for day-one taking into account advice from the STAP. The aim was a scope upgradable to full specifications as they were defined in the instrument proposal. Cost: 18 M€
- 3. A configuration where the instrument is in the full technical scope. This is a refined scope presented in the proposal [1], taking into account changes in the ESS design during Phase1 and advice from the STAP. Cost: 27.3 M€

1.4. Basic project timeline

The timeline for the instrument construction is organised with the intention to be in the operation programme among the first instrumentsin the first half of 2023. Most of the periods will need time overlaps. The reason is, for example, expected overbooking of the guide manufacturers or availability of installation ground. This will be difficult at the point of the management and Tollgate reviews and readiness reports.

Staging to full-scope specifications will depend on the funding schedule and resources available during the hot commissioning and initial operation period. Details need to be communicated with ESS management.

2. OPTION 1: INSTRUMENT WITHIN THE COST CATEGORY B (12M€)

2.1. Scope

- the bi-spectral extraction system
- S-shape curved guide expanding after the first kink and blocking the direct line of sight for the first time inside the bunker wall
- sample position at 157 m
- 1 Modulation Chopper and one frame overlap chopper
	- \circ Single disk rotating at ~9 m
	- o Single disk rotating at ~80 m
- two detectors at ±90° with the size of 50 cm x 50 cm and resolution of 5 mm x 5 mm fixed at 2 m from the sample using $10B$ technology with a single set of radial collimators
- sample positioning: 2t load table (z, omega), linear stages for xyz
- sample environment: only pool sample environment
- all necessary associated infrastructure (shielding, cabling, control hutch, etc.)
- smaller instrument cave 8 m x 7 m and a limited load of the platform
- no transport system for long-term experiments and user sample environments between the elevated instrument cave and the laboratories on the ground floor.

This scope does **not** meet the top level requirements for:

- limited sample environment not directly dedicated for engineering research (#2)
- limited sample complexity, maximal load and throughput (#3)
- microstructure except macrostrain (#4)
- long-term experiment support (#5)
- \bullet d-range (#6)
- pole figure coverage (#7)
- texture evolution (#8)
- limited gauge volume by one set of radial collimators (#12)
- d-resolution (#14)
- weight limited to 2 t (#16)
- \bullet SANS (#17)

The science case for BEER is mainly based on in-situ and in-operando experiments. Since only experiments with ESS pool sample environments would be possible, the instrument capability

would be severely downgraded. Only part of the planned engineering specific SE could be delivered during staging period because of the reduced cave and user lab areas.

The small detector coverage has three major negative consequences:

- 1. The detector coverage of 0.5 x 0.5 $m²$ is below the present-day standard and sets back the envisaged improvement in data acquisition rate due to the high source brightness as it was pointed out by the STAP
- 2. Monitoring of texture evolution during in-situ experiments may not be possible. For a complete pole figure, the sample has to be rotated around several axes, which can be impossible in many cases due to the constraints which are given by sample environment and required strain components.
- 3. Without the low- and high-angle detectors, the d-range accessible simultaneously in one measurement would be significantly reduced and become insufficient for studies of present or future advanced engineering materials.

The chopper system only assumes the modulation method, which is well suited for mapping residual strains in materials with high crystallographic symmetry but is much less suited for studying the evolution of multiphase materials during in-situ tests. Together with missing instrument flexibility in selection of resolution modes, this would seriously reduce the scope of research and user community the instrument could address. Studies of materials exhibiting significant peak broadening effect due to microstrains could probably not be carried out at BEER, in contrast to the existing instruments.

This scope is only upgradeable with high additional costs since no placeholders are foreseen for the additional choppers. At least the initial 5 m of neutron guide in the bunker, as well as the detectors, would have to be replaced. This variant also assumes much smaller and simpler instrument cave and experimental platform, which doesn't allow future extension of detector coverage (including SANS) and accommodation of engineering specific sample environment suite.

Therefore, BEER would not be competitive in a major part of its research scope to the existing world class instruments.

This scope **does not fulfil** the science case proposed for BEER.

2.2. Costing

The strategy for setting the scope of BEER within the cost category B was to deliver an instrument capable of at least some engineering types of experiment. Due to the mandatory expenses for the long neutron guide, shielding, and reasonable detector coverage the engineering dedicated sample environment had to be severely reduced. It was therefore not possible to satisfy any of the science drivers presented in the proposal. Hence the cost category instrument is a simple, non-competitive and expensively upgradable engineering instrument with a largely reduced scientific scope. The costing is based on an assumption of the procurement costs and manpower required to deliver the high-level PBS items. Vacuum equipment and DMSC items are not included in the cost as these are expected to be delivered outside of the BEER budget.

Table 1 Costing for BEER in Cost Category B

2.3. Upgrade/Staging plan

The staging plan to full scope makes a re-build of the instrument cave and the platform necessary to be able to accommodate additional detectors, such as the SANS detector, and allow the handling of the heavy and large samples or sample environments. Re-build of the instrument cave can be problematic due to complicated interface between neighbouring instruments. Furthermore, the staging consists of replacing the small detectors by larger ones and moving the smaller ones to the detector arc or other in-plane positions. Guide segments in the bunker have to be redesigned and replaced to fit in additional choppers (PSC's, MC's and FC's). Access to the bunker will be only possible during target shut-down within the highly risk environment what makes upgrade even more time-consuming and more costly. All those updates are very expensive and time-consuming operations which make the staging to the full scope unrealistic for this cost category scope. Therefore, a detailed staging plan has not been developed.

2.4. Risk

The main risk for this configuration is the failure in delivering the top-class instrument which can match the science case presented to the SAC for the day-one. This scope represents the instrument which is below the performance of existing engineering instruments, and STAP found this configuration inadequate as stated above. Upgrade to the full scope is almost impossible without severing reconstruction or re-build of crucial parts as neutron guides within the bunker or the instrument cave which is timely and costly.

Below are top 5 risks rated high using ESS risk measures (impact x likelihood).

Table 2 Top 5 risks for Option 1

3. OPTION 2: WORLD CLASS INSTRUMENT (18 M€)

3.1. Scope

- bi-spectral extraction system
- S-shape curved guide expanding after the first kink and blocking the direct line of sight for the first time inside the bunker wall
- guide exchanger with two focusing options (without multichannel focusing)
- sample position at 157 m
- two modulation choppers, three pulse shaping choppers (1 movable) and two double disk frame overlap choppers
	- \circ one double disk rotating at ~9 m
	- o three single disks rotating at \degree 6.5 7.6 m
	- \circ one double disk rotating at \sim 8.3 m
	- o one double disk rotating at 80 m
- two detectors at ±90° using ¹⁰B technology with the size of 100 cm x 100 cm and resolution of 2 mm x 5 mm at 2 m from the sample but moveable between 2 and 3 m for placing voluminous samples and sample environment
- sample positioning: 3t load table (z, omega), linear stages for xyz, robot, hexapod
- sample environment: advanced stress rig with vacuum furnace, pool sample environment
- all necessary associated infrastructure (shielding, cabling, control hutch, etc.)
- docking platforms for long-term experiments, user sample environments and easy transportation between instrument cave platform, ground level and engineering and/or preparatory laboratory
- big instrument cave 12 m x 10 m with an elevated platform to hold the heavy sample and/or sample environment and accommodate SANS detector in an upgrade phase

This scope does **not** meet the top level requirements for:

- not full sample environment suite (#2)
- \bullet d-range (#6)
- pole figure coverage (#7)
- texture evolution (#8)
- \bullet SANS (#17)

This scope aims at delivery of a world class instrument able to yield excellent results in some of the proposed research areas since day-one and thus to ensure early success of the project. The scope is proposed so that it is possible to upgrade the instrument to the full specifications described in the original instrument proposal in a staging process.

The scientific scope covered by this instrument is similar to the existing engineering instruments. This is a world class instrument assumed to outperform existing instruments for example in the broad resolution/intensity range that can be offered, including the unique modulation method for high-flux/high-resolution regime. The detector coverage is comparable to the present state-of-the-art instruments like ENGIN-X or TAKUMI. Due to the missing arc detectors, the sample has to be rotated in several directions to cover a full pole figure. However, these detectors can be added to the staging plan during first years of operation. The same is applicable for the additional SANS detector and third modulation chopper which enable simultaneous SANS and diffraction measurement.

This scope includes an advanced deformation rig with the maximal force of 60 kN equipped by vacuum chamber and furnace with resistive and induction heating systems. The development of an ultra-high temperature furnace (temperatures up to 1500°C) for this deformation rig is planned in collaboration with user community (proposed project in collaboration with Chalmers University and Technical University of Stockholm), and it should also be available for the day-one experiment.

Thus, the scope of the World Class instrument does match most of the science case described in the BEER proposal and already before staging to the full specification is comparable with or in some aspects already outperforms the present state-of-the-art instruments.

3.2. Costing

Costing strategy and calculations are based on procurement cost and manpower required for delivery of the instrument with the specifications given above. The cost calculation includes mandatory parts for day-one operation such as neutron guides, shielding, choppers and basic detectors. Upgradable parts as sample environment, additional detectors, SANS option, etc. are postponed to the staging plan. Vacuum equipment and DMSC items are not included in the cost as these are expected to be delivered outside of the BEER budget.

	01 Phase 1	02 Project Management & Integration	03 Design	04 Procurement & Fabrication	05 Installation	06 Cold Commissioning	Total
01 Shielding	€0	€0	€0	€ 2.543.726	€476.672	€0	€3.020.398
02 Neutron Optics	€0	€0	€0	€ 2.791.000	€ 0	€0	€ 2.791.00
03 Choppers	€0	€46.200	€0	€ 1.860.000	€ 55.080	€ 29.580	€ 1.990.900
04 Sample Environment	€0	€0	€0	€ 330.000	€ 0	€0	€ 330.000
05 Detector Beam and Monitors	€0	€0	€0	€ 2.888.900	€0	€0	€ 2.888.900

Table 3 Costing for BEER Option 2

Date 2016-10-04

3.3. Upgrade/Staging plan

The staging process is planned to increase the performance in subsequent steps reflecting STAP recommendations. The staging can be divided into two parts: (i) upgrade of the instrument and (ii) upgrade of the sample environment (SE) suite.

The instrument upgrade staging consists of following steps (in order of importance):

- 1. add horizontal 1×1 m² detector at -130 $^{\circ}$
- 2. add arc detectors
- 3. add backscattering detector
- 4. add horizontal 1×1 m² detector at 50 $^{\circ}$
- 5. add SANS option

Both additional horizontal detectors will cost about 2,405 k€ while the arc detectors cost was evaluated to 2,163 k€ including three 0.5x0.5 m² detectors with radial collimators fixed on an arc-portal. Funding sources are not yet clear and have to be identified before staging process starts. The additional cost for the modulation chopper MCc will be 217 k€ and will come in combination with the SANS option which will cost 1,399 k€ including detector and vacuum tube.

Additionally, SE will be staged following the STAP recommendation (order can be changed if external funding source can be identified and/or preferences of user community preferences change):

- 1. biaxial stress rigs (rotation + uni-directional or bi-directional deformation)
- 2. digital image correlation
- 3. annealing furnace for engineering samples
- 4. welding devices (laser, friction stir)
- 5. Gleeble simulator

3.4. Risk

The main risks for this configuration are delays in delivery of various ESS systems and BEER components, especially the neutron guides and shielding. High risk is also in possible underestimation of shielding costs because sufficiently accurate MC simulations and cost estimates will be possible only during and after the detailed engineering design phase. Another risk is the lack of funding sources for upgrades in the staging period.

Below are top 5 risks rated high using ESS risk measures (impact x likelihood).

4. OPTION 3: FULL SCOPE INSTRUMENT

4.1. Scope

- bi-spectral extraction system
- S-shape curved guide expanding after the first kink and blocking the direct line of sight for the first time inside the bunker wall
- guide exchanger with three focusing options
- sample position at 157 m
- 3 Modulation Choppers, 3 Pulse Shaping Choppers (1 movable) and two double disk frame overlap choppers
	- \circ one double disk rotating at ~9 m
	- o one single disk rotating at ~9.5 m
	- \circ three single disks rotating at \sim 6.5 -7.6 m
	- o one double disk rotating at ~8.3 m
	- o one double disk rotating at 80 m
- Four detectors at $\pm 90^\circ$, -130° and 50° using ¹⁰B technology with size of 100 cm x 100 cm and resolution of 2 mm x 5 mm at 2 m from the sample but moveable between 2 and 3 m for placing voluminous SE
- backscattering detector with the size of 50 cm x 50 cm and resolution of 5 mm x 5 mm at 1.5 m
- three detectors with size of 50 cm x 50 cm and resolution of 2 mm x 5 mm placed on the off-plane arc construction at 90° equipped with radial collimators and with sampledetector distance 1.2 m
- sample positioning: heavy load table, linear stages for xyz, robot, cybaman, hexapod
- sample environment: advanced stress rig with vacuum furnace, dilatometer, pool SE
- all necessary associated infrastructure (shielding, cabling, control hutch, etc.)
- universal platform for long-term experiments, user sample environments and easy transportation between instrument cave and engineering laboratory
- big instrument cave 12 m x 10 m with an elevated platform to hold the heavy sample and/or sample environment

This scope meets all the high-level requirements and fulfils the science case presented to SAC.

4.2. Costing

The costing is based on calculations of the procurement costs and manpower required for the tasks needed to deliver the full scope BEER instrument and is presented in following table split into the higher level PBS items. Vacuum equipment and DMSC items are not included in the cost as these are expected to be delivered outside of the BEER budget.

	01 Phase 1	02 Project Management & Integration	03 Design	04 Procurement & Fabrication	05 Installation	06 Cold Commissioning	Total
01 Shielding	€0	€0	€ 0	€ 2.543.726	€476.672	€0	€ 3.020.398
02 Neutron Optics	€0	€0	€ 0	€ 2.891.000	€0	€0	€ 2.891.00
03 Choppers	€0	€ 50.320	$\boldsymbol{\epsilon}$ 0	€ 2.065.000	€ 59.940	€ 32.190	€ 2.207.450
04 Sample Environment	€0	€0	€ 0	€ 1.130.000	€0	€0	€ 1.130.000
05 Detector and Beam Monitors	€0	€0	€0	€9.068.750	€0	€ 0	€9.068.750
06 Data Acquisition and Analysis	€0	€0	€ 0	€0	€0	€0	€0
07 Motion Control and Automation	€0	€0	€ 0	€96.100	€49.660	€ 0	€ 145.760
08 Instrument Specific Technical Equipment	€471.850	€993.000	€947.100	€ 1.845.100	€ 670.500	€439.200	€ 5.366.750
09 Instrument Infrastructure	€0	€0	€ 0	€ 780.000	€0	€0	€780.000
10 Vacuum	€0	€0	€ 0	€0	€0	€0	€0
11 PSS	€0	€0	$\boldsymbol{\epsilon}$ 0	€ 177.000	ϵ 0	€0	€ 177.000
12 Contingency							€ 2.478.711
Total	€471.850	€1.043.320	€947.100	€ 20.596.676	€ 1.256.772	€471.390	€ 27.265.819
Labour included in above (Person- Years)	3.1	5.5	$6.8\,$	2.0	6.5	3.8	27.7

Table 5 Costing for BEER Full Scope

4.3. Upgrade/Staging plan

Further development of the instrument would be most probably focused on the sample environment specific to material engineerings, such as the Gleeble simulator or specialised devices for in-operando measurements designed and constructed in collaboration with the user community.

4.4. Risk

The main risks for this configuration are delays in delivery of various ESS systems and BEER components. This option has a higher detector coverage and thus the likelihood of a delay in detector delivery is greater. It is also probable that installation and integration of the rich sample environment suite will have to continue during the hot commissioning phase due to the lack of manpower and interference with the early operation plan.

Below are top 5 risks rated high using ESS risk measures (impact x likelihood).

Table 6: Risks for Option 3

5. REFERENCES

- 1. ESS Instrument Construction Proposal <<Beamline for European materials Engineering Research (BEER)>>
- 2. Concept of Operaton Document 13.6.6 BEER.docx