

Concept of Operations for Polarized Reflectometer (Estia)

Version 1.2

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1 Introduction

1.1 Purpose of the document

The purpose of this ConOps is to provide a brief description of the *Estia*, the polarized reflectometer for small samples. The description includes both a high level introduction to the science case of the instrument as well as providing the framework and context within which the instrument will be designed, operated and maintained through its life-cycle. The intended audience for this document includes everyone involved in the construction and operation of *Estia*. It will also serve the function as a quick overview of the instrument's purpose, construction and operation for both person/-s familiar in the field of neutron science and those that are not.

1.2 Definitions, acronyms and abbreviations

Abbreviation	Explanation of abbreviation
PNR	Polarized Neutron Reflectometry
SLD	Scattering Length Density – The physical property defining the neutron contrast for reflectivity from thin films
TG	Tollgate
VS	Virtual Source

2 Science Case

The following is a short summary of the *Estia* science case to put the instrument into perspective. A detailed description can be found in chapter 1 of the *Estia* proposal.

2.1 Introduction

Physical, chemical and biological states or processes at interfaces and surfaces become increasingly important in fundamental and applied science. This field extends from improving surface conditioning or understanding biological mechanisms at cell membranes, to the improvement of magnetic data storage and processing, and the investigation of novel phenomena when conflicting properties are forced to coexist on an atomic scale.

One of the best suited methods to investigate interfaces is reflectometry, where the intensity and direction of a beam reflected on a surface is detected as a function of incident energy and orientation. It provides the depth-profile (specular reflectometry) as well as information about lateral inhomogeneities of structure (off-specular reflectivity and grazing incidence small angle neutron scattering GISANS).

Neutron reflectometry (NR) in particular provides a high penetration depth, sensitivity also for light elements, allows for contrast variation by isotope substitution and it probes magnetism. Accordingly, the neutron reflectometry user community and therefore also the demands to the instruments are quite broad.

Typical systems under investigation include:

- Layers with exchange-bias effects between ferro- and anti-ferromagnets
- Multiferroic materials with simultaneous magnetic and electric order
- Ion diffusion in solids as that of Lithium in battery materials
- Gas condensation on cold surfaces, e.g. formation of spontelectric films
- Cell membrane shape changes due to electric field
- Ordered magnetic nanoparticles with considerable dipole-dipole interaction
- Magnetic layers with strong spin-orbit coupling producing e.g. Skirmion vortex states

- Artificial spin-ice systems with macroscopic magnetic frustration
- Self-assembly of surfactants, polymers and proteins at solid and solid-liquid interfaces
- Rearrangement processes in thin films: e.g. interdiffusion, inter-layer movement
- Encapsulation and release of components in e.g. plastics, polymer blends, drug delivery
- Switchable materials that respond to external stimuli (chemical, electrical, magnetic, optical)
- Surface reactions e.g. enzyme catalysis, oxidation, surface functionalization etc.
- High-throughput screening of e.g. biological/medical samples or industrial conditions

In the following sections the special design criteria for *Estia*

- sample size,
- measurement time,
- resolution and q_z -range,
- lateral structure, and
- polarization
- diffraction capability

are presented together with scientific examples and a discussion of the performance of *Estia* in this respect. For clear understanding it is essential to be aware of *Estia*'s unique features: the guide delivers a beam of a wide divergence, strongly focused to the sample. The footprint and the divergence of the beam incident on the sample is defined independently from each other by special diaphragms far before the sample. The focusing limits the maximum footprint height of the beam on the sample to ≈ 10 mm. The angular resolution is solely provided by the area-sensitive detector. To allow for a combination of bulky sample environment and high detector angles, the scattering geometry is horizontal.

2.2 Small size

The driving design criterion for *Estia* was to be able to measure on small samples, or on small selected areas. Small here means below $10 \times 10 \text{ mm}^2$ down to $1 \times 1 \text{ mm}^2$, much smaller than what is possible at other instruments right now. The maximum footprint of *Estia* is $\approx 10 \times 50 \text{ mm}^2$.

Currently many NR experiments are prohibited by the limited surface area of interesting samples. Reasons for this include limitation in sample fabrication, time consumption to provide sufficient amount of material, the cost of constituents, limited size of substrate crystals and optimization to other characterization methods.

An additional aspect of the *Estia* optics is the ability to define the beam footprint on the sample far away from the sample position. This allows experiments with e.g. electrical contacts to be performed without simultaneously measuring covered areas of the sample. In addition, samples can be placed within bulky sample environment without compromising the instrument performance.

As this definition of beam footprint size and divergence is a unique feature of *Estia*, a high priority is given to its performance and sample environment equipment like sample holders, cryostat and liquid-solid cells will be optimized for small sample sizes.

2.3 Measurement time

The peak flux gain of the ESS compared to existing neutron sources and its efficient use by *Estia* will reduce the measurement time by at least one order of magnitude. Another order can be gained for moderate size to small samples by using *Estia*'s unique high-intensity specular reflectivity mode.

This aspect will allow the instrument to perform standard experiments in reduced time and screen an extended physical parameter space. Additional possibilities include time resolved and spectroscopic studies.

To make full use of these advances fast sample changes and time resolved measurements as a function of external parameters have to be taken into account in the design of the instrument components.

2.4 Resolution and q_z -range

As described in section 2.1 the *Estia* science case includes a large variety of phenomena and sample systems with different experimental difficulties and structural length scales. To be able to cover all these cases the instrument has to cover a large enough q_z range and allow for moderate as well as high resolution measurements. For most specular

reflectometry experiments the relevant lengthscales are between 1 nm and 100 nm with critical edges close to 0.01\AA^{-1} . A relative resolution of $\frac{\sigma q_z}{q_z} \leq 3\%$ and a q_z -range from 0.005\AA^{-1} to 0.6\AA^{-1} is sufficient to measure these systems.

With access to high intensity neutron beams much smaller structures (few \AA) as for example multilayers of membranes, self organized lipid layers and interfacial magnetism at oxide interfaces become accessible. To be able to measure these important systems, access to 1\AA^{-1} is often required. This large q_z experiments not only necessitate sufficient incident intensity and angular detector range but a low enough instrument and sample specific background to be able to reach reflectivities down to 10^{-7} - 10^{-8} . While for hydrogen containing liquid-solid samples the sample specific background is dominated by spin incoherent scattering, which is directly proportional to the solid angle of the detector area integrated when extracting the specular reflectivity, many experiments on solid substrates and with extended sample environment suffer from the strongly structured signal of multiple Bragg-scattering from the substrate crystal and neutron windows. To get rid of this diffraction it is necessary to move the incident wavelength band above the relevant Bragg-edges (e.g. 4.6\AA , 6.2\AA , 7\AA , 7.8\AA , and 8.6\AA for Al, Si, Al_2O_3 , SrTiO_3 , and Quartz respectively).

In cases of specialized samples as liquid-solid cells and to allow better quantification of unknown SLD films it can be necessary/advantageous to perform reflectometry from both sides of the substrate-film interface. For this capability it is necessary to move the detector to negative scattering angles. The signal to background in this experiments often limits the accessible q_z -range, thus a maximum q_z of -0.3\AA^{-1} will be sufficient.

Although of less importance than the above mentioned use cases, an option for high resolution measurements is desirable to be able to resolve very thick layers as well as Kiessig fringes of multilayers with a large number of repetitions. Especially for investigations of interface effects on atomic scale such multilayers will still be necessary to reach sufficient signal at the large q_z values of interest and the additional global information from the Kiessig oscillations help to pin down variations of the bilayers throughout the whole sample. A relative resolution of $\frac{\sigma q_z}{q_z} \leq 1\%$ will be sufficient for this application.

2.5 Laterally structured systems

The ability to measure off-specular scattering and later possibly GISANS gives additionally access to in-plane structures on the film surface or buried within the film. Examples of this include magnetic structures like domains and nanoparticles as well as correlated wiggles in lipid membranes.

Due to the long projection of the incident and out-going neutron wave vector onto the substrate surface the length scales probed with off-specular scattering and GISANS are intrinsically much different. It is therefore desirable to allow both experiments with

sufficient off-specular q -range and GISANS resolution to probe the full range of sizes with sufficient overlap. With the same incident beam parameters in both directions the GISANS measurement has the same resolution in q_y as is available in reflectometry for q_z . Considering that sufficient intensity may necessitate a relaxation of the resolution a reasonable upper size limit for GISANS would be 50 nm, a typical size for nanoparticle assemblies. To be able to measure this length scale with off-specular scattering a q_x range of 0.02\AA^{-1} is desirable.

2.6 Polarization

The neutron magnetic moment is a perfect probe for magnetism. For reflectometry, polarized neutrons and neutron polarization analysis allow depth resolved vector magnetometry for a broad range of materials.

In non magnetic layer systems, magnetic substrates are often used for so called magnetic contrast variation, which allows to emphasize different aspects of the system.

While polarization efficiency for diffraction measurements needs only to be moderate ($\approx 90\%$) the difference in reflectivity for different spin-states can often be more than an order of magnitude. For this reason the measurement sensitivity is strongly limited by the amount of cross-talk from the other spin-states and a much better polarization $\geq 95\%$ must be provided.

2.7 Diffraction capability

There are many thin film systems where the effects of scientific interest are caused by multi-scale structures. For example the anti-ferromagnetic order in a multiferroic material, molecule alignment of lipids or atomic arrangement in spontelectric films are directly linked to the macroscopic behavior. Today this necessitates neutron reflectometry and diffraction experiments to be carried out subsequently, which is not only problematic for samples which need to be deposited shortly before the experiment but often delays publication of the results. Although *Estia* will not be optimized for diffraction experiments the high neutron flux at ESS will allow measurements with similar quality as can be done now at other sources. This will not only allow to combine two very different experiments within one proposal but more importantly allow screening for such short range effects before performing a full diffraction study on a different beamline.

From an instrument development point of view a coverage of a larger q -range has the additional benefit to allow access to high quality crystal Bragg-peaks as Si-(111), which can be used to quantify the precision of the time of flight of the measurement and the wavelength resolution function.

3 System Characteristics

3.1 System purpose

The *Estia* instrument is a vertical sample reflectometer with polarization analysis optimized for small, solid samples. To allow the measurement of down to $\leq 1 \text{ mm}^2$ sample surface with sufficient intensity it is based on the focusing reflectometry[1] principle using a *Selene* neutron guide[2]. *Estia* will primarily serve the hard condensed matter community as complimentary instrument to the horizontal sample reflectometer *FREIA*, providing a larger q-range and sample environment for diverse magnetic experiments to ESS. For more details on the scientific case see chapter 2 and the *Estia* Instrument Proposal.

3.2 System Life-Cycle

The figure below shows the life-cycle of the *Estia* instrument with the corresponding further detailed development phases. Each phase of the instrument development is concluded with a TG review, with accompanying design review. During one phase, construction and installation, there will be an intermediate design review – TRR.

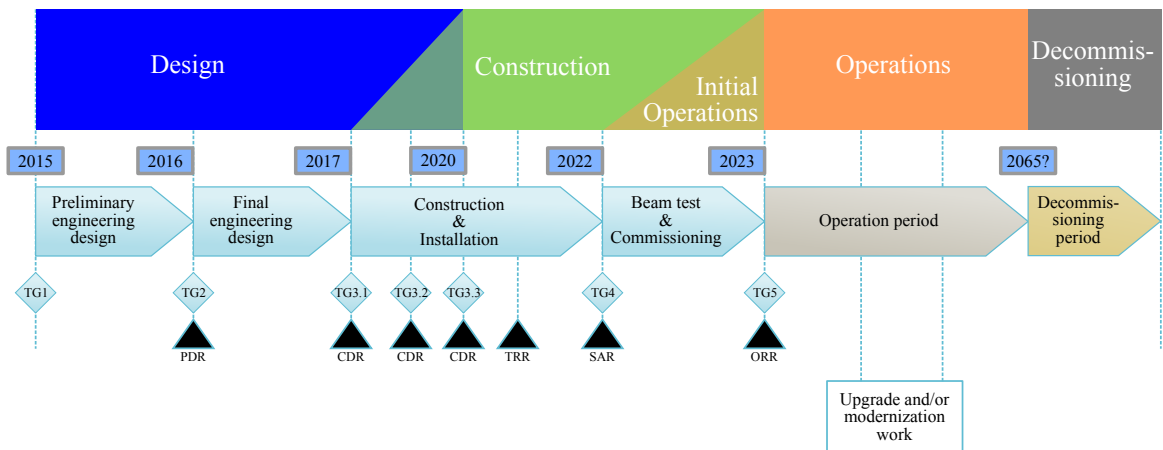


Figure 3.1: *Estia* life cycle

The overall life-cycle stages are:

Design stage aims to develop the instrument from the proposal to a build ready state, with a majority of design drawings and component sourcing finalized, fulfilling all requirements. To ascertain that the instrument maturity progresses as planned two TGs, with accompanying design reviews, are conducted. PDR is the Preliminary Design Review and CDR is the Critical Design Review. As the instrument consists of several fairly separated work packages the availability of manpower as well as tight schedule will be dealt with by splitting the CDR into three separate instances to allow beginning of construction before the independent work package detailed design is finished.

Construction stage aims to deliver a fully built, verified, tested and commissioned, ready for full operations, instrument. The stage is split into two phases; the construction & installation and the beam test & commissioning, where each phase is concluded with a toll gate and accompanying design reviews. SAR – Safety Assessment Review and ORR – Operational Readiness Review. For the construction & installation phase another design review is conducted; TRR – Technical Readiness Review. The TRR is conducted to ensure that the instrument can proceed to and successfully conduct the SAR.

Operations stage aims to maintain an instrument with high availability and reliability for the user community to perform experiments. The operations stage will allow for scheduled maintenance as well as periods where upgrading and/or modernization of *Estia* can be done. With upgrade it is meant that additional functionality/capability is introduced and with modernization enhancement of existing functionality is implemented.

Decommissioning stage this is the period where the instrument shall be dismantled and disposed of in a safe a controlled manner, adhering to all radiation safety requirements. It is possible that *Estia* will be decommissioned before ESS has reached its own decommissioning stage.

3.3 System Overview

The *Estia* instrument concept is a focusing, vertical sample, time-of-flight reflectometer with full polarization analysis capability and large detector angle. In contrast to typical neutron reflectometers, the focusing reflectometry principle uses a wide beam divergence in both directions and analyzes the reflection angle with the position sensitive detector. For a suitable application of this approach to small samples a beam with good focusing on the sample position is required, which can be provided with the *Selene* neutron guide concept, a set of two elliptical neutron guides that compensate for the most dominant aberration effects. For the *Estia* concept the *Selene* guide is doubled in vertical direction, producing two separate beams that are guided to the sample position, although initially

only the Feeder will be build with two sets of mirrors to allow later upgrade of the instrument.

In addition to providing a large divergence on a small sample area this concept can be used to image a "Virtual Source" aperture placed before the first ellipses onto the sample, allowing control of illumination and divergence far away from the sample. This aspect is of great advantage for many solid states experiments as large sample environments can be used while controlling the neutron beam footprint on the sample.

An overview about the important *Estia* components is given in Figure 3.2:

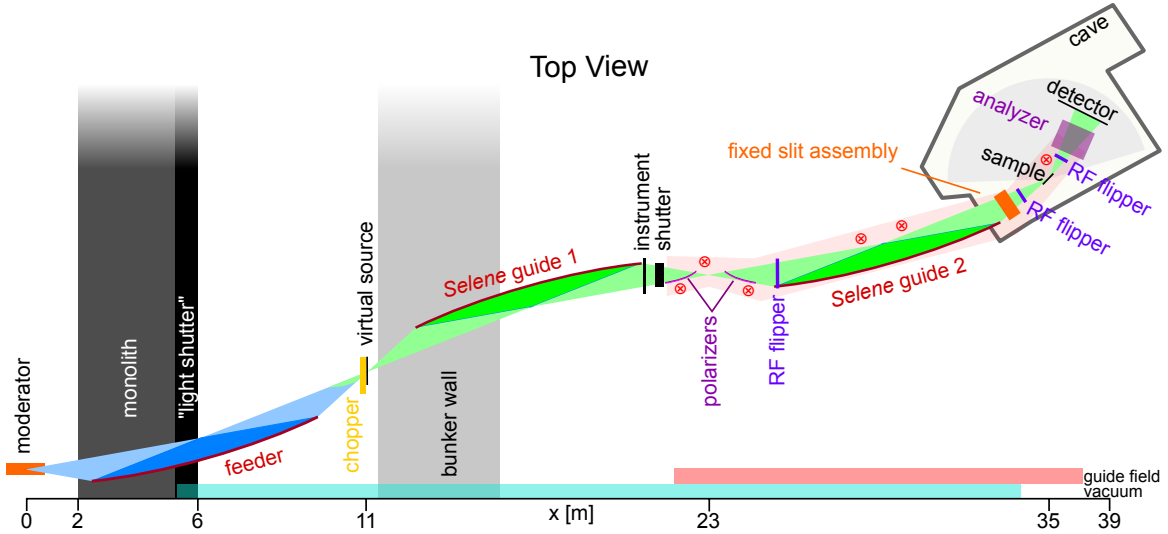
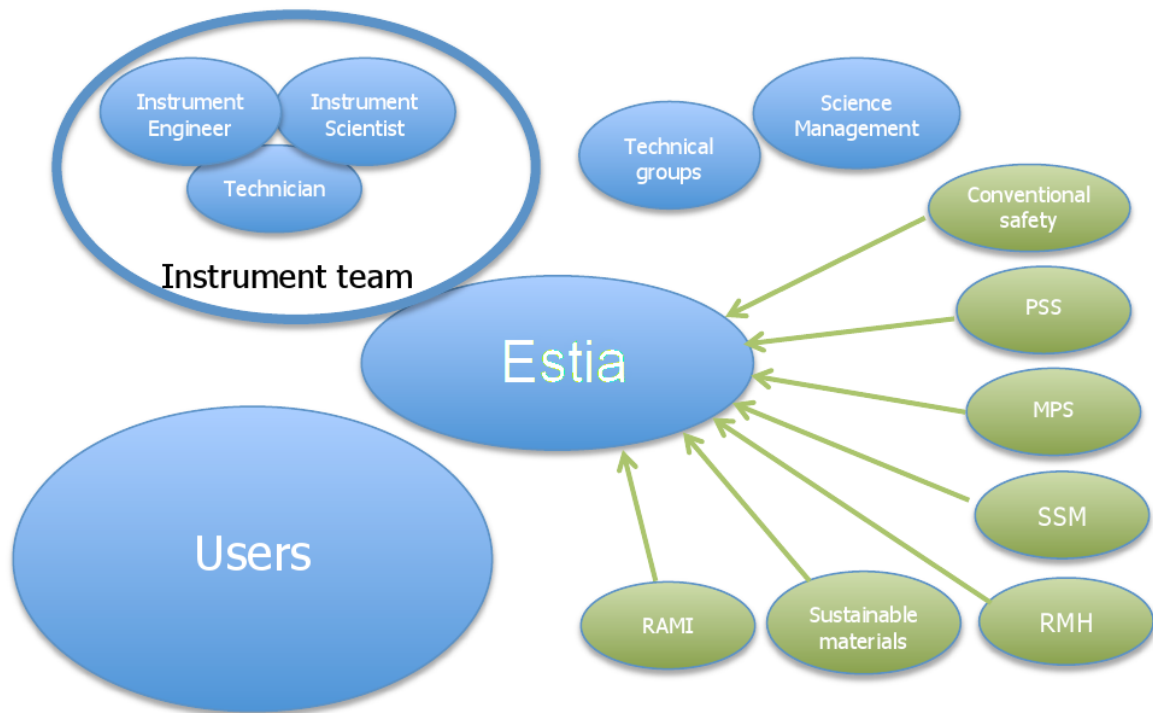


Figure 3.2: *Estia* instrument overview

The neutron beam from the cold source is guided to the VS using a set of elliptical mirrors referred to as *Feeder*. This mirror needs to be separated into two parts, inside and outside the monolith, to allow closing of the monolith light shutter system. A set of movable absorbers is positioned in the second focus of the feeder, defining the beam shape of the VS. The neutron bandwidth is defined by a disc chopper directly in front of the VS.

Further downstream the two *Selene* guides transport the beam to the sample cave. In the middle focus, between the two *Selene* guides, the instrument shutter and two logarithmic spiral shaped polarizing supermirrors are places. The second *Selene* guide enters the experimental cave, which houses several beam shaping options, the sample positioning stack and sample environment as well as a detector arm with polarization analyzers and position sensitive detectors. As the polarizers, the analyzer mirrors are of logarithmic spiral shape, reflecting the divergent beam after the sample in vertical direction. With this geometry the reflected spin-up component and transmitted spin-down component can both be measured at different areas of the detectors. The two separate vertical beams have each a dedicated detector.

4 System Stakeholders



The most important group of stakeholders is the users. The scientists who already use neutron reflectometry in their research will be able to do more and more challenging experiments. In the very large group of scientists who use X-ray reflectometry, many will have the possibility to use also *Estia* with their thin films of interest, thus gaining new insight. Samples prepared for other investigation techniques, often limited in size to $<5 \times 5 \text{ mm}^2$, will be measurable with *Estia* that are not accessible with current neutron instruments. The scientific partners are in the forefront of the general user community and through their early involvement in the project they will be able to make full use of the instrument from the beginning.

The value to the ESS stakeholders is firstly that a scientifically excellent instrument will be delivered to the ESS user program in cost and schedule. The instrument will contribute to the overall scientific impact of the ESS and help make ESS a success. For the ESS technical groups it is important that the technical components of the instrument can be maintained in a sustainable manner.

Group ID	Stakeholder Group	Individual ID	Stakeholder	Surrogate	Interest in the project	Actions by instrument team
SH-1	User community	SH-1.1	Existing neutron reflectometry users	STAP	Access to a worldleading instrument, perform experiments not possible elsewhere	Regular reporting to the STAP, participation in topical conferences, dissemination of instrument progress
SH-1	User community	SH-1.2	X-ray reflectometry and other thin film technique users	STAP	Access to a new method to answer scientific questions	Participation in relevant meetings, dissemination of instrument progress
SH-2	PSI	SH-2.1	Instrument core team	SPL (Artur Glavic) LE (Sven Schütz)	Instrument delivered within budget and in schedule to hot commissioning, merit for career development	Regular meetings and tight coordination within the core team and other PSI groups
SH-2	PSI	SH-2.2	Optics and shielding team	GL (Uwe Filges) PD (Christine Klauser)	Instrument delivered with low background, development of novel neutron optics, merit for career development	Regular meetings for optics and shielding discussions
SH-3	ESS	SH-3.1	Instrument construction subproject	CIPE (Gabor László) SIPA (Ken Andersen)	World leading instrument delivered to hot commissioning, instrument construction project delivered in schedule and budget	Regular meetings, timely reporting
SH-3	ESS	SH-3.2	Neutron scattering systems project	NSS PM (Shane Kennedy)	Suite of world leading instruments delivered within schedule and budget, integration with technology development and supporting facilities	Timely reporting when requested
SH-3	ESS	SH-3.3	Science Directorate	DS (Andreas Schreyer)	Instrument ready to produce scientific results early on, high scientific impact for facility	Timely reporting when requested
SH-3	ESS	SH-3.4	Neutron Optics Group	GL (Philip Bentley)	Good instrument performance, standardization across instruments	regular meetings, ensuring coordination and integration with the rest of the instrument
SH-3	ESS	SH-3.5	Neutron Chopper Group	GL (Iain Sutton)	Good instrument performance, standardization across instruments	regular meetings, ensuring coordination and integration with the rest of the instrument

Group ID	Stakeholder Group	Individual ID	Stakeholder	Surrogate	Interest in the project	Actions by instrument team
SH-3	ESS	SH-3.6	Detector Group	GL(Richard Hall-Wilton)	Good instrument performance, standardization across instruments	regular meetings, ensuring coordination and integration with the rest of the instrument
SH-3	ESS	SH-3.7	Electrical Engineering Group	GL (Thomas Gahl)	Good instrument performance, standardization across instruments	regular meetings, ensuring coordination and integration with the rest of the instrument
SH-3	ESS	SH-3.8	Scientific Activities Division	DH (Arno Heiss), Zoë Fisher	Scientifically productive instrument, serve the user community	Communicate sample and support facility requirements clearly
SH-3	ESS	SH-3.9	DMSC	GL (Thomas Holm Rod)	Scientifically productive instrument, serve the user community	Regular meetings, clearly communicated requirements

5 Operational Concepts

5.1 Operational environment

Following the baseline for beamport allocation *ESS-0047786 Estia* as a short instrument will be located in the east sector on port E02 within the experimental hall 1 with building designation D01. Figure 5.1 shows the instrument location within the experimental hall.

The hall will be operated in a controlled environment with a temperature of $22\pm 2^\circ\text{C}$ all year around. The floor height in experimental hall 2 is 2 m below target centerline. Free height to lifting hook of the overhead gantry crane is maximum 7 m in the experimental hall. Floor loading in the experimental hall must not exceed 20 T/m^2 . Floor underneath the bunker can accommodate a loading of up to 30 T/m^2 . Floor stability in the hall is specified to be maximum 4 mm w.r.t elastic movement and another maximum 4 mm due to creep/deformation. Utilities and media are brought to the instrument from the gallery. Media include: DI- H_2O , N_2 , instrument grade compressed air, cooling water low. Utilities include: office IT, office comms, Power, MPS, PSS, DMSC and ICS. For detailed and updated listing of requirements and/or 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 suggested solution could be to place ventilation hoods directly above instrument equipment generating most heat. This, in-turn, could have an impact on selection of location of such equipment and thus considerations for this need to be made. For the most sensitive components of *Estia* an active, local temperature control is envisioned.

The ESS facility has 5 different operating modes, ref *ESS-0003640*: Shutdown, Studies, Studies on Target, Startup and Production. These modes have various impact on instrument operations. Pure experimental work can only be conducted during ESS-mode Production. Access to instrument equipment for maintenance, calibration, cold commissioning is mainly done during shutdown, studies and studies on Target – naturally after due safety assessment and still possibly with some restrictions. During start-up instrument operations is limited to alignment, commissioning and calibration runs.

When ESS has entered into a steady-state operations phase the following principal schedule will apply:

- 200 days/year of neutron Production for the ESS users after 2026,

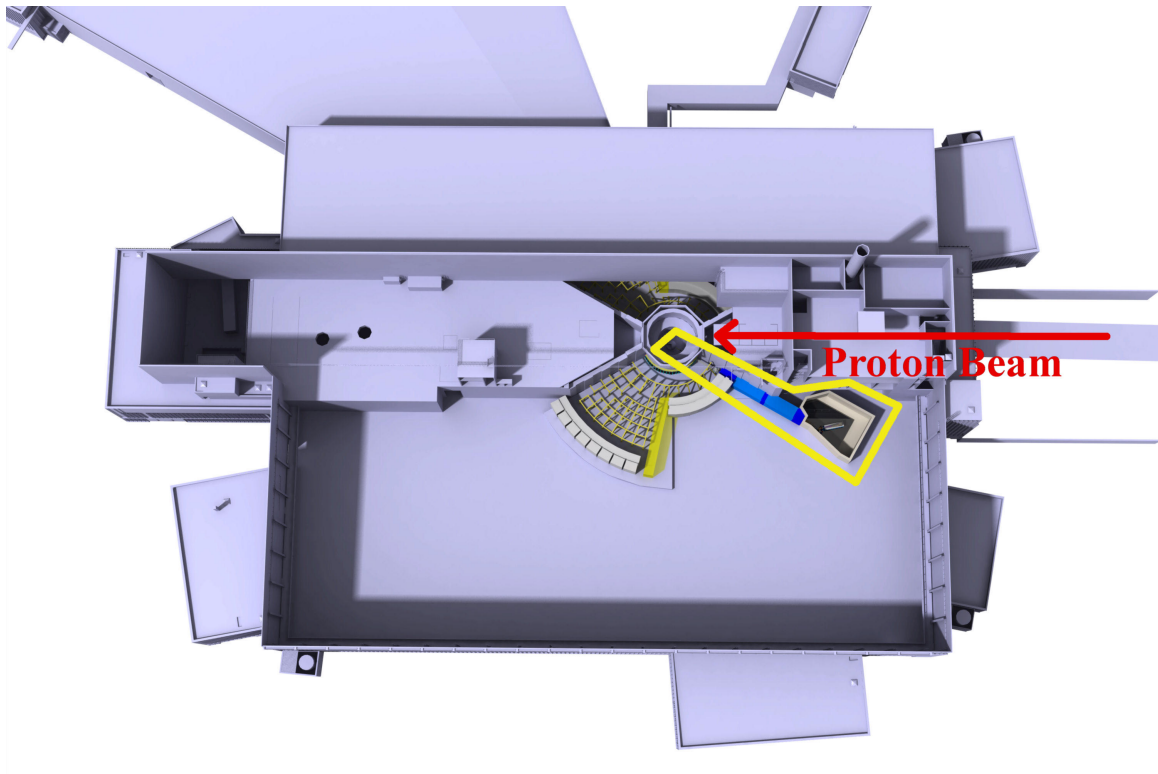


Figure 5.1: Envisioned location of *Estia* at port E02

- 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 down time 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 to the availability and reliability assessments made in ref *ESS-0017709* and *ESS-0008886*.

The *Estia* instrument is foreseen to be managed and operated by a team of 3-4 scientists and at least one engineer, which may be several shared appointments. ESS will be manned 24 hours/day, not all categories, but this manning will allow for flexibility for users when conducting experiments and making preparations or analyzing results. At the instrument team's and users' disposal for data collection, storage and analysis are the tools provided by DMSC, physically located in Copenhagen. If the allocated average beamtime at *Estia* will be smaller than 3 days it will be challenging, even for 3 scientists

to properly support users with data analysis, so dedicated on-site staff with this expertise will be necessary.

5.2 Operational scenarios

Streamlining of the user and sample changing process is of crucial importance for the long-term scientific productivity of the instrument. Most experiments performed at *Estia* will be carried out within a limited range of physical parameters, namely non-ambient temperatures and moderate magnetic fields. Therefore instrument specific closed cycle refrigeration and an electromagnet will be permanently installed at the instrument. This specialized equipment will be optimized for quick sample change and off-instrument sample preparation as short measurement times for standard experiments are foreseeable. A well defined interface will be provided at the beamline to, in addition, accommodate ESS pool sample environment for a broad range of physical property manipulation.

The beamtime for user experiments is allocated in a peer-review process based on scientific merit and feasibility. Proprietary access for industry is also envisaged, but likely of minor importance in the *Estia* case.

Typical users of the *Estia* instrument will be chemists, physicists and material scientists working with thin solid films with varying experience in reflectometry techniques. Supporting hardware and software will be implemented to allow even inexperienced users to measure and change samples and physical parameters after a short (<1 h) introduction by the ESS instrument team. As data analysis from reflectometry requires some degree of expertise it is expected that a considerable amount of users will need support either by the ESS instrument team or a dedicated DMSC expert. The user team would typically consist of 1-4 scientists (PhD level or doctoral students) who perform the experiment within the allocated beamtime. They either bring their samples with them, ship them beforehand, or prepare them using the ESS supporting facilities.

The users will process the data at the ESS by at least up to a point where it can be input to third party software. For focusing reflectometry this means a proper normalization and binning of the raw time-of-flight data into R vs. Q datasets.

Reflectivity experiments are performed on thin films with single layer thicknesses in the order of 1-100 nm. Mostly, these films are deposited onto single crystal substrates with rectangular surface and 0.3-1 mm thickness. *Estia* will provide a set of standard sample holders with various sizes, where samples are mounted on a flat surface either with some kind of adhesive or with vacuum pumped holes. Standardization of these sample holders will allow prealignment of samples outside the instrument to quickly begin the experiment after a sample change. The ESS instrument team will assist users in the first mounting processes.

Once mounted the sample will be exposed to the neutron beam and the reflected neutrons detected with a position sensitive time-of-flight detector. The detected data, often using several angles of incidence, together with previously measured reference datasets can then be processed by instrument specific software to produce a reflectivity curve.

5.2.1 Conventional ToF reflectometry and off-specular scattering mode

When the incident beam is horizontally collimated with a conventional slit the measurement can be carried out exactly as is done with time-of-flight reflectometers at various other facilities. This mode allows to record off-specular scattering together with the specular information and there are no additional challenges involved in the data collection or analysis.

5.2.2 High intensity specular reflectometry mode

In this mode the full beam divergence is incident on the sample and the position sensitive detector is used to separate the different reflection angles. The intensity gain to the conventional mode is about one order of magnitude, which makes it the optimal setting to measure very small samples or fast, time dependent effects.

With the expected flux for the *Estia* instrument the measurement times in this mode can be extremely short, sometimes below 1 min per reflectivity curve. There are several scenarios envisioned, where this will be applied to standard experiments, all of which need to be considered in the instrument operation.

Large amount of samples To quickly screen a large set of samples the sample position for room temperature measurements will accommodate a vacuum sample holder for fast changes and simple linear translation to simultaneously attach several samples. A quick alignment will be facilitated by a special alignment laser system.

Magnetic field scans The instrument control software will allow a continuous change in external field while measuring, that can later, during data reduction, be selectively split into reflectivity curves for the desired field regions. The same principle can be applied for other external parameters like electric field.

Temperature sweeps The laser alignment system will allow in-situ control of the sample position to keep it positioned within the neutron beam focus while sweeping temperature and thus allowing similar experiments with changing temperature.

Low temperature sample changes An optional multiple sample holder will be attachable to the refrigerator, to allow the measurement of several sample while only cooling them down once.

5.2.3 Background suppression and GISANS mode

Using a refocusing device in front of the sample, the vertical divergence can be directed to the detector. This mode can be used with larger samples to improve the intensity to background ratio or to measure Grazing Incidence Small Angle Neutron Scattering to access in-plane surface structures in the sample. From the users perspective, there is no additional complexity to such measurements compared to the conventional mode.

5.2.4 Neutron polarization

Although the hardware requirements some aspects of the data reduction software are considerably different from the unpolarized operation of the instrument, the user experience does not differ from what is described above. The separately recorded spin channels, either by measuring with and without spin-flipper or by separation with the analyzer mirror onto different areas on the detector, each correspond to distinct reflectivity curves.

5.2.5 Other sample environment

In addition to measuring in low temperatures and magnetic fields, *Estia* will allow experiments with a large variety of sample environment equipment, as the important optical components all are situated far away from the sample area. Electric fields will be applied with ESS pool equipment, using fixed installed wiring at the instrument. High temperature will be made available within the closed cycle system using a Sapphire insulated sample holder or, for higher temperatures, a ESS pool sample furnace. Possibilities to operate shared specific equipment with *FREIA* (e.g. liquid flow cells) will be available.

5.3 Maintenance Concepts

5.3.1 Levels of maintenance

Within ESS there are three identified levels of maintenance, see ref *ESS-0003640*:

1. Organizational maintenance: maintenance performed on site where the element 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 term supplier includes In-Kind partners.

5.3.2 Maintenance categories

Maintenance can be divided into two categories: Corrective and Preventive. By utilizing 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 minimize disruption to user operation.

Preventive maintenance is part of scheduled maintenance which also include maintenance work to be conducted on equipment where condition based monitoring cannot be achieved. Performed instrument reliability analysis, part of RAMI work, should aim to ascertain that preventive maintenance on this type of equipment/components could be limited to periods of scheduled shutdown of the facility.

During scheduled maintenance access to components that are within e.g. common shielding bunker will require a cooling period before they are safe from a radiological view to handle.

Some components, (i.e detectors) can be maintained without removing them from their installed position, but other (e.g. chopper) will have to be removed for maintenance. To remove a component typically requires that the surrounding radiation shielding (including the common bunker shielding for components within the bunker) is either removed or opened by a hall or local crane. The time taken for removing the shielding is often a major part of the maintenance time and crane availability may become limiting, particularly for the work that can only be done after the proton beam has been off target for a sufficient time. The removed shielding elements have to be stored in the hall during the maintenance time. When the maintenance is completed the shielding has to be replaced and its radiological integrity verified by e.g. an interlock procedure.

Some of the component maintenance can be done on site, but some components may have to be sent to manufacturers, which incurs a longer lead time, but also imposes stricter radiological constraints as the equipment has to leave the site.

The components requiring more frequent maintenance include constantly moving parts such as choppers, vacuum pumps etc. The maintenance schedule will be developed to ensure a minimal need for unscheduled maintenance (see 5.3.3) and consequent loss of user beamtime. As the lead time for maintenance varies strongly depending on the position of the component, the components in less easily accessible locations have less frequent maintenance. Corrective maintenance will mainly apply when an event happens forcing maintenance to be done unscheduled. This occurs when either a component failure or detection of an issue that requires immediate action during user operation. The instrument will have to stop user operations for the duration of repairs or maintenance. The unscheduled maintenance of components that are not accessible when the proton

beam is on target will have to wait for the next facility shutdown, which may cause significant loss of beamtime.

To minimize this type of maintenance a great deal of consideration needs to go into the design of each piece of equipment of the instrument to facilitate for swift and safe corrective measures to be made, to the greatest extent possible. Another design goal for key components of *Estia*, that are not accessible during facility operation, is to allow a (probably limited scope) operation of the instrument even after such hardware fails. This includes for example a chopper failure to only occur in the open state and a mechanism to move a broken virtual source out of the neutron beam.

5.3.3 Maintenance philosophy

Estia 's maintenance philosophy aims to utilize condition based preventive maintenance as much as possible. In order to minimize time spent and increase efficiency when performing maintenance, inspectability and accessibility are two features requiring a good deal of attention in the design work. In general, access to instrument equipment along the beam guide shall be from the top, especially in the bunker region. In this area the aim is to utilize remotely operated vehicles to do the maintenance work, to the greatest possible extent. Further downstream as the allocated beam line sector widens more space will be available facilitating access from the sides for inspection and maintenance.

Outside the bunker area the shielding concept is designed to allow access to most of the beamline equipment even during normal neutron production at ESS.

6 Consequences of the Concept

6.1 General design considerations

6.1.1 Upgrade options

During the development work identified upgrade options shall be considered and be catered for if possible in the design solutions. These options include, but are not limited to, a second detector for the down directed part of the vertically split beam, a refocusing option in front of the sample, a second CCR for faster sample changes and a in-situ sample growth chamber.

6.1.2 Robust design

Due to the hostile environment along the entire beamline, in particular inside the target monolith insert and the common shielding bunker area, design solutions should be made as robust as possible. Robust should be regarded in terms of e.g. minimizing number of components, moving parts (reducing maintenance efforts) and maximizing structural strength. Robust design solutions should also support the ability, where possible, to enable a degraded performance mode in case a failure or an unintentional misalignment occurs.

Robust design applicability could include:

- Chopper design
- Virtual source system
- Neutron feeder
- Monolith light shutter – extraction for feeder out of shutter and closing of shutter

Mitigating measures elsewhere along the beamline should be investigated should some of the issues/problems above occur.

6.2 Coordination with other systems

Close monitoring and continuous coordination with the following interfacing systems is critical:

- Neighboring beamlines – especially the first 12 m from target center. Compromises cannot be ruled out possibly affecting design and performance of the *Estia* instrument. This should be kept in mind and possible scenarios of how to mitigate such compromises should be considered. Outside the bunker space monitoring of allocated space is mainly required for the *Selene* mirror mounting system and various expected maintenance activities.
- Target monolith insert – optics alignment, cooling solution, The insert is provided by Target System to NSS design specification
- Light shutter – optics alignment, position repeatability and beam guide gap. The light shutter is provided by Target System to NSS design specification and adapted to *Estia* specific needs
- Bunker system – alignment components in the bunker, optics insert in bunker wall. The bunker is provided centrally by NSS based on requirements from the instruments
- Feeder – components of neighboring instruments have to be taken into account to avoid interference with the movable feeder components (e.g. wide choppers)

6.3 Training of personnel

The organization for operating instruments at ESS is yet to be decided. The team would likely include at least three instrument scientists who are knowledgeable in polarized neutron reflectometry and can translate scientific needs to technical requirements. The instrument scientists have to maintain a research profile and dedicate time to scientific research in order to understand the needs of the 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 would include mechanical, electrical, software and other specialty engineer and technician personnel, who could be part of the instrument team and/or in specialized technical groups.

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 ESS instrument team and the less experienced users, who would require more support, would be expected to establish a collaboration with ESS scientists.

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Referenced ESS Documents

ESS-0047786 Baseline for ESS Beamport Allocation

ESS-0008886 ESS Reliability and Availability requirements

ESS-0003640 ESS Concept of Operations Description

ESS-0017709 Experiments expected at ESS and their neutron beam needs