

Estia - System Requirements

Version 1.2

	Name	Affiliation
Authors	Artur Glavic, Sven Schütz	PSI
Reviewers	Jorgen Andersson Phil Bentley Thomas Gahl Francesco Piscitelli Hanna Wacklin	ESS ESS ESS ESS ESS
TG2 Review Committee	Shane Kennedy (Chair) Ken Andersen John Ankner Robert Cubitt Sylvain Désert Richard Hall-Wilton Arno Hiess Gábor László Iain Sutton	ESS ESS STAP STAP LLB ESS ESS ESS ESS
Approver	Andreas Shreyer	ESS

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European Spallation Source ESS AB
 Visiting address: ESS, Tunavägen 24
 P.O. Box 176
 SE-221 00 Lund
 SWEDEN
www.ess.se

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1 Introduction

1.1 Purpose of the document

This document describes the functional requirements for the subsystems of the focusing polarized neutron reflectometer *Estia*. These requirements are based on the high level scientific requirements derived from the scientific case of the instrument as outlined in the instrument proposal as well as in the Concept of Operations (ConOps) document that describes the expected operational use of the instrument. The subsystem requirements in this document are based on the conceptual design presented in the instrument proposal.

1.2 Definitions, acronyms and abbreviations

Abbreviation	Explanation of abbreviation
PBS	Product breakdown structure
BTCS	Beam transport and conditioning system
SES	Sample exposure system
SCS	Scattering characterization system
PNR	Polarized Neutron Reflectometry
VS	Virtual Source
SE	Sample Environment
PSS	Personal Safety System
BPA	Baseplat Position Accuracy
DMSC	Data Management and Software Center
DAQ	Data Acquisition
ToF	Time of Flight

Specific to neutron guides:

Abbreviation	Explanation of abbreviation
segment	A single physical piece of a neutron guide as produced by the vendor.
mirror	A collection of segments that belong to the same geometrical shape or serves the same physical purpose. An example would be an elliptical mirror, which describes one reflector with elliptic shape that is implemented using several segments.
guide	One or more mirrors that share the same location on the beam axis and form one component of the beam delivery system. An example would be an elliptical guide that is a collection of four elliptical mirrors, two opposite mirrors for horizontal and vertical direction, each.
guide system	The collection of neutron guides that form the full beam delivery system from source to sample.

2 System Characteristics

2.1 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.

2.2 System overview

The instrument consists of three main technical subsystems: the beam transport and conditioning system (BTS), the sample exposure system (SES) and the scattering characterisation system (SCS). In addition, as described in the instrument product breakdown structure (PBS), the instrument includes the structures that house and support these subsystems, the software to control the instrument and the software to process the data. The hardware description in this document does not strictly follow the PBS, but rather a functional breakdown of technical components along the neutron beam path. This makes it easier to map the specifications to the high level scientific requirements. PBS numbers are given for reference where appropriate.

2.3 High level system requirements for the Instrument (13.6.9)

From the scientific requirements described in the ConOps document section 2 the following high level system requirements are derived:

Req. #	Description
13.6.9r1	The instrument shall allow specular reflectivity measurements from samples between 1x1 mm ² and 10x10 mm ² .
13.6.9r2	The instrument shall cover a q_z range from 0.005Å ⁻¹ up to 1Å ⁻¹ with wavelengths above 8Å.
13.6.9r3	The instrument should allow inverse reflection geometry up to a negative q_z of 0.02Å ⁻¹ .
13.6.9r4	The instrument shall provide a typical relative resolution of $\frac{\sigma q_z}{q_z} \leq 2.5\%$.
13.6.9r5	The instrument should provide a high resolution option for $\frac{\sigma q_z}{q_z} \leq 1\%$, not limited by the detector resolution.
13.6.9r6	The instrument shall provide neutron polarization analysis with polarizations >95% over the whole wavelength and divergence range.
13.6.9r7	The beam size at the sample position shall be controllable to minimize over illumination and concentrate on specific sample areas.
13.6.9r8	The instrument should provide options for the measurement of off-specular and Grazing Incidence Neutron Scattering.
13.6.9r9	The instrument should minimize the background from high energy neutrons and other non-sample intrinsic sources.
13.6.9r9.1	<i>Estia</i> shall be able to measure the reflectivity of 20 nm Nickle on a 10x10 mm ² Silicon substrate down to 10 ⁻⁶ initially.
13.6.9r9.2	<i>Estia</i> should be able to measure the reflectivity of 20 nm Nickle on a 10x10 mm ² Silicon substrate down to 10 ⁻⁷ after hot commissioning.
13.6.9r9.3	Using the high intensity mode, <i>Estia</i> should be able to measure the reflectivity of 20 nm Nickle on a 1x1 mm ² Silicon substrate down to 10 ⁻⁵ after hot commissioning.
13.6.9r10	The instrument should allow fast sample changes within ≈10 min or less.

In the list above and all following requirements the prefix σ refers to the standard deviation of a value and δ to the full width at half maximum (FWHM). For a Gaussian distributed value the values can be converted with a factor $\delta \approx 2.35\sigma$, while for nearly uniform distributed values as the time of flight resolution the conversion factor is $\delta \approx 3.46\sigma$. (Δ values describe parameter ranges, not accuracy.)

While the instrument specific background is a very important aspect of developing a neutron reflectometer it is hard to quantify. For the purpose of the instrument construction and validation the subrequirements have therefore been included in the list above.

3 Beam Transport and Conditioning System (13.6.9.1)

The beam transport system transports a beam of neutrons from the moderator surface to the sample. The size, divergence and wavelength spectrum of the beam are tailored to the needs of the experiment. In particular the selected wavelength band and source to detector distance allow measurements with the desired resolution starting at the wavelength of highest intensity (4Å). The natural time resolution of ESS ($\delta t \approx 3$ ms) with the source to detector distance of 39 m at 4Å allows a relative q-resolution of $\frac{\sigma q_z}{q_z} \approx 2.3\%$ (FWHM $\frac{\delta q_z}{q_z} \approx 8\%$).

3.1 Neutron Guides

3.1.1 Supermirror coating

The coating requirements are given by the wavelength range accessible by the instrument and the specific angles of impact on the mirrors. While the neutron guides would require different m-values at different positions, this variation is small and will not lead to increased cost when replaced by one fixed value. For the polarization devices the smallest accessible q needs to be considered in addition to larges one, as the polarization is only available in this range. Here the values are chosen to allow an efficient polarization of the full available neutron band while, at the same time, being able to use the natural silicon reflectivity for frame overlap filtering.

Req. #	Parameter	Description	Value/Error
13.6.9.1r1	m_{Feeder}	Supermirror coating for the elliptical guides (Ni/Ti)	4
13.6.9.1r2	m_{Selene}	Supermirror coating for the elliptical guides (Ni/Ti)	4
13.6.9.1r3	$m_{Polarizer}$	Supermirror coating for the transmission polarizers (Fe/Si)	5
13.6.9.1r4	$m_{Frame-Overlap}$	Coating for the frame-overlap mirrors (plane Si)	-
13.6.9.1r5	$m_{Frame-Overlap2}$	Coating for the frame-overlap mirrors use in case of chopper failure (Ni/Ti)	1.8

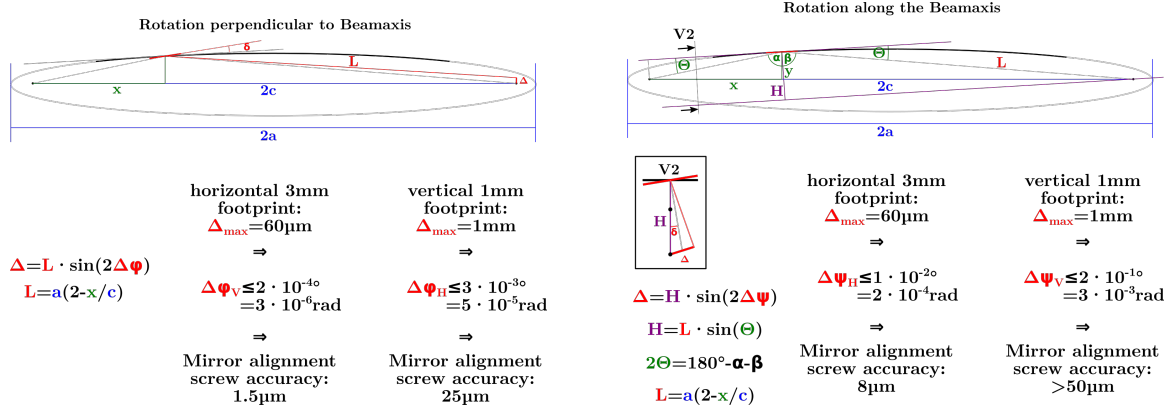


Figure 3.1: Geometrical derivation of necessary alignment precision of *Selene* guide segments to properly image a $60 \mu\text{m} \times 1 \text{mm}$ slit.

3.1.2 Guide segment alignment

The most challenging task for the neutron optics is to image a well defined footprint from the VS to the sample surface. To make full use of this technique a footprint of 3mm length and 1mm height will allow to measure selective areas of samples without illumination of unwanted parts as for example electric contacts. In addition this allows to keep the amount of over illumination in standard experiments and with it the background produced by the direct beam to a minimum. Due to the small incident angle of the sample in PNR this translates to approximately $60 \mu\text{m}$ beam width at the sample (at 1.2° incident angle). Using geometrical considerations this can be translated into angular alignment precision of the neutron guide segments as is shown in figure 3.1. The shown ranges are the result for the calculation at different positions of the ellipses.

Translational offsets of the segments are only of minor importance to this consideration, as they only lead to a small reduction of transmitted intensity. The requirements for the *Feeder* are more relaxed, as the image of the source projected onto the VS is much bigger then the slit itself. Therefore the values are taken for 1mm maximum offset, which corresponds to the alignment precision of the cold moderator and is therefore the limit of maximum precision reasonably desirable.

3.1.3 Neutron Feeder (Beam Extraction System 13.6.9.1.1))

Req. #	Parameter	Description	Value/Error
13.6.9.1r6	<i>Feeder :</i>	Alignment precision of the neutron feeder optics segments to each other	
13.6.9.1r6.1	δn_V	Vertical mirror position offset in direction normal to surface	50 μm
13.6.9.1r6.2	δp_V	Vertical mirror position offset in direction parallel to surface	200 μm
13.6.9.1r6.3	$\delta \phi_V$	Vertical mirror surface with respect to rotations around the vertical axis (z).	$3 \cdot 10^{-3}^\circ$
13.6.9.1r6.4	$\delta \psi_V$	Vertical mirror surface with respect to rotations around the beam axis (x).	$2 \cdot 10^{-1}^\circ$
13.6.9.1r6.5	δn_H	Vertical mirror position offset in direction normal to surface	50 μm
13.6.9.1r6.6	δp_H	Vertical mirror position offset in direction parallel to surface	200 μm
13.6.9.1r6.7	$\delta \phi_H$	Horizontal mirror surface with respect to rotations around horizontal axis (y).	$3 \cdot 10^{-3}^\circ$
13.6.9.1r6.8	$\delta \psi_H$	Horizontal mirror surface with respect to rotations around beam axis (x)	$2 \cdot 10^{-1}^\circ$

3.1.4 Selene Neutron Guide (Beam Delivery System 13.6.9.1.2))

In addition to the requirements listed below the system design should include means to measure the alignment of the individual guide segments to the necessary precision.

Req. #	Parameter	Description	Value/Error
13.6.9.1r7	<i>Selene :</i>	Alignment precision of the <i>Selene</i> optics segments to each other	
13.6.9.1r7.1	δn_V	Vertical mirror position offset in direction normal to surface	50 μm
13.6.9.1r7.2	δp_V	Vertical mirror position offset in direction parallel to surface	200 μm
13.6.9.1r7.3	$\delta \phi_V$	Vertical mirror surface with respect to rotations around the vertical axis (z).	$2 \cdot 10^{-4}^\circ$
13.6.9.1r7.4	$\delta \psi_V$	Vertical mirror surface with respect to rotations around the beam axis (x).	$2 \cdot 10^{-1}^\circ$
13.6.9.1r7.5	δn_H	Vertical mirror position offset in direction normal to surface	50 μm
13.6.9.1r7.6	δp_H	Vertical mirror position offset in direction parallel to surface	200 μm
13.6.9.1r7.7	$\delta \phi_H$	Horizontal mirror surface with respect to rotations around horizontal axis (y).	$3 \cdot 10^{-3}^\circ$
13.6.9.1r7.8	$\delta \psi_H$	Horizontal mirror surface with respect to rotations around beam axis (x)	$1 \cdot 10^{-2}^\circ$

3.1.5 Relative alignment of components to each other/to hall

The precision requirements given in the previous sections all refer to one elliptical system and relative positioning of neutron mirror segments to each other. These values are far more restrictive than the absolute alignment of the components to each other, as a rotation or translation of one ellipses to the other in first order only leads to a change in sample position, no broadening of the focus point. The following requirements describe the individual assembly total positioning and take into account vertical drift due to floor sinking:

Req. #	Parameter	Description	Value/Error
13.6.9.1r8	Δv_{adj}	Minimum adjustment range of components in vertical direction.	± 15 mm or BPA
13.6.9.1r9	δv_{adj}	Alignment precision for vertical adjustment.	0.1 mm
13.6.9.1r10	Δh_{adj}	Minimum adjustment range of components in horizontal direction.	± 5 mm or BPA
13.6.9.1r11	δh_{adj}	Alignment precision for horizontal adjustment.	0.1 mm

3.2 Choppers (13.6.9.1.3)

For the *Estia* concept the focusing optics and polarization requirements limit the usable wavelength range on both the short- and long-wavelength side. The guide transmission for very long wavelength is strongly reduced due to gravity and very short wavelength need larger polarizing supermirrors and higher m-value coating for all guides. In addition the need for a very broad wavelength band is reduced due to the large Θ coverage available. The intrinsic resolution of the ESS pulse at the expected detector position at ≈ 40 m from the source is sufficient for most reflectivity experiments.

Therefore no complex beam shaping or frame multiplication scheme is required and a single 14 Hz band width chopper between the feeder and bunker wall can be used. The chopper size should be chosen appropriate for the beam diameter, so that the opening/closing times are smaller than 2 ms. In this configuration the bandwidth is $\Delta\lambda = 6.9\text{\AA}$ and the relative resolution $\frac{\delta\lambda}{\lambda}$ varies from 7.5% at 4\AA to 2.7% at 11\AA . The first contamination with longer wavelength starts above 29\AA and is only transmitted with very low intensity through the *Selene* guide. The remnant intensity shall be suppressed with a frame overlap mirror or the polarizing supermirror, dependent on the configuration.

To expand the usable wavelength band for single shot experiments the chopper should be able to allow frame skipping mode operation, i.e. it should be operable at 1/2 and 1/3 of the source frequency.

Req. #	Parameter	Description	Value/Error
13.6.9.1r12	$f_{Chopper}$	Beam chop frequency	14 Hz/7 Hz/ $4\frac{2}{3}$ Hz
13.6.9.1r13	$t_{O/C}$	Chopper opening/closing times for full beam	<2 ms
13.6.9.1r14	$\Delta\lambda$	Bandwidth of the instrument	6.9Å
13.6.9.1r14.1	λ_{range}	Available wavelength range accessible with different chopper phases	3Å-25Å
13.6.9.1r15	$\delta\lambda$	Wavelength resolution, given by pulse length and detector distance	0.3Å
13.6.9.1r15.1	$\frac{\delta\lambda}{\lambda}$	Relative resolution	<8%

3.3 Beam Geometry Conditioning (13.6.9.1.4)

3.3.1 Virtual Source (Aperture Collimation System 13.6.9.1.4.3.1)

The virtual source (VS) is a set of vertical and horizontal neutron absorbers, that allow the definition of the sample footprint as it is imaged through the Selene guide system onto the sample. It is positioned in the common focus of the neutron Feeder and Selene guide 1 within the bunker. To be able to define the footprint as desired from the reflectivity geometry the absorbers shall allow to define the vertical height of the beam, length of the sample in beam direction and incident angle on the sample, which also acts to open the slit size. As the sample footprint can be very small horizontally the VS absorbers need to be very precise and the translational motion needs to keep the vertical edges of the absorbers as parallel as possible. The values listed below are based on the same footprint estimations as described in section 3.1.

For alignment purposes the VS should also contain one or more precise circular apertures that can be moved into the beam instead of the slit opening.

Req. #	Parameter	Description	Value/Error
13.6.9.1r16	h_{max}	Maximum slit size in vertical direction	20 mm
13.6.9.1r16.1	Δh_{center}	Available range to adjust vertical center position	± 2.5 mm
13.6.9.1r17	δh	Positioning accuracy for vertical motion	0.1 mm
13.6.9.1r18	l_{max}	Maximum slit size in beam direction	50 mm
13.6.9.1r18.1	Δl_{center}	Available range to adjust horizontal center position	none
13.6.9.1r19	δl	Positioning accuracy for horizontal motion	0.1 mm
13.6.9.1r20	ω_{max}	Maximum VS rotation angle around vertical axis	10°
13.6.9.1r21	$\delta\omega$	Accuracy of rotational motion	0.05°
13.6.9.1r22	δd_{10}	Maximum horizontal size variation of slit over 10 mm beam height. Needs to be preserved after horizontal and vertical size changes.	$10 \mu\text{m}$

3.3.2 Middle focus aperture system (13.6.9.1.4.3.2)

For instrument alignment and verification purposes there shall be a changeable set of apertures at the focus between Selene guide 1 and 2. At least the following absorbers shall be present:

Req. #	Description
13.6.9.1r23	Circular aperture with different sizes to analyze Selene guide 2 imaging quality
13.6.9.1r24	Horizontal and vertical single slits for one directional analysis
13.6.9.1r25	Large rectangular aperture to remove neutrons not imaged onto the sample position

3.3.3 In-cave optical components

After the exit of Selene guide 2 a vacuum area shall be provided for neutron beam shaping optical components. These components can be inserted into the beam to operate the instrument in different modes or for alignment purposes.

Beam shaping slit system (13.6.9.1.4.5) To operate in almost-conventional reflectometry, off-specular or GISANS mode the divergence of the beam shall be controllable with a motorized slit system after the Selene guide 2 exit. The accuracy and geometry of the system must allow a full beam opening and a closing in both directions to achieve good angular resolution. To fulfill the best resolution requirements at the lowest q_z

defined in section 2.3 for 11Å (0.25° incident angle) the standard deviation must be smaller than 0.0025°, which is 0.0087° FWHM for a slit.

Req. #	Parameter	Description	Value/Error
13.6.9.1r26	$\delta\theta_h$	Minimum resolution achievable with the slit system in horizontal direction	0.005°
13.6.9.1r27	$\Delta\theta_h$	Minimum full opening of the slit system in horizontal direction	2.0°
13.6.9.1r28	$\delta\theta_v$	Minimum resolution achievable with the slit system in vertical direction	0.02°
13.6.9.1r29	$\Delta\theta_v$	Minimum full opening of the slit system in vertical direction	5.0°

Space-time collimator (moving aperture) [upgrade option] For extended q-range almost-conventional reflectometry and off-specular scattering as well as for fixed \vec{k}_i GISANS measurements a system of movable absorbers at different distances from the sample shall be provided as an option with coupled motion to the source frequency. With such a system it is possible to change the incident angle on the sample coupled to the incident wavelength and thus measure with a collimated beam but at the same time make use of the available horizontal divergence to extend the q-range at fixed sample position. By having these absorber blades at different distances one can, in addition to the definition of the incident angle, use the space-time collimator to increase the wavelength resolution as with a similar chopper setup.

Req. #	Parameter	Description	Value/Error
13.6.9.1r30	f_{STC}	Space-time collimator repetition frequency.	14 Hz
13.6.9.1r31	$\Delta\theta_{STC}$	Horizontal angular coverage to be accessible by the blade	1.5°
13.6.9.1r32	$\frac{\delta\lambda_{STC}}{\lambda_{STC}}$	Horizontal angular coverage to be accessible by the blade	1.5°

Refocussing mirror [upgrade option] An optional neutron supermirror shall be provided to allow to refocus the vertical beam divergence from the sample position onto the detector. This option will allow a high resolution, high intensity GISANS mode and the reduction of incoherent background from the sample by integrating over a smaller detector area.

Req. #	Description
13.6.9.1r33	Refocussing mirror needs to fit within the in-cave optics vacuum system
13.6.9.1r34	Vertical focus distance needs to be changed by 4 m to converge at the detector position

Ultra-precise focusing [upgrade option] The small focus of *Estia* will enable, for the first time, efficient imaging experiments with microscopic magnification. Although the $<60\ \mu\text{m}$ horizontal focus will not achieve better than state of the art imaging performance, it allows access to a demanded size regime with a novel approach and possible neutron polarization analysis.

As an optional enhancement for these kind of experiments and reflectivity measurements with higher demands on footprint control, the instrument should be equipped with a focus enhancement optics. This can be achieved by reflecting the beam coming from the second half Selene guide 1 onto the second half of Selene guide 2, reaching a focus size 3x smaller than with the normal setup. A second refocussing mirror in the in-cave optics region can be used to move the focus closer to the guide and decrease its size even further this way.

Req. #	Description
13.6.9.1r35	Reverse refocussing mirror needs to fit within the in-cave optics vacuum system
13.6.9.1r36	Horizontal and vertical focal distance needs to be minimized
13.6.9.1r37	Flat mirror at middle focus needs to have high m-value and alignment mechanism

3.4 Beam Filtering System (13.6.9.1.5)

The following explanations are the basis for the requirements listed in section 3.1.1.

3.4.1 Frame Overlap Mirror (13.6.9.1.5.2)

The requirements of the frame overlap mirrors are the same as for the neutron polarizers when removing the polarizing supermirror coating. An optional second set of frame overlap mirrors should be provided with increased m-value to be use in case of chopper failure. This second set should restrict the wavelength band to $<11\text{\AA}$ and this way allow a normal operation of the beamline even without a bandwidth chopper. (Short wavelength are cut by the transmission of the neutron guide.)

3.4.2 Neutron Polarisation System (13.6.9.1.5.3)

The polarizers shall not impact the imaging quality of the Selene guide system, therefore it most likely will be a transmission polarizing supermirror. The mirror coating shall be chosen to allow polarization of the full bandwidth in normal operation ($4\text{-}11\text{\AA}$). A full polarization of the second frame ($11\text{-}18\text{\AA}$) is desired, as it allows to measure with polarized beam even in pulse skipping mode. On the low q side the polarizer should also

act as a frame overlap mirror, cutting neutrons above 29Å. In addition the coating shall fulfill the polarization requirements of >95% stated in section 2.3.

These boundary conditions are met using two subsequent passes through an Fe/Si supermirror transmission polarizer coated on a silicon substrate. For 4Å at m=4.5 typical single pass polarization is >90%, leading to >99% for two transmissions. In this configuration 29Å reflects at m=0.62 and is cut by the natural supermirror critical edge. This also allows the usage of single layer coated silicon wavers as frame overlap supermirrors.

3.4.3 Neutron Spin Flippers (13.6.9.1.5.4)

For full polarization analysis a radio frequency (RF) spin-flipper before and after the sample shall be present. If technically feasible, the separate definition of each of the vertical beams would be desirable.

Req. #	Description
13.6.9.1r38	RF flipper in front and after sample position
13.6.9.1r39	Flipper efficiency for main band >99%
13.6.9.1r40	If feasible, additional flipper for just one vertical beam before sample

3.4.4 Neutron Spatial-Spin-Resonance Flipper [upgrade option]

To allow high resolution measurements an option shall be provided to use a spacial-spin-resonance flipper to increase wavelength resolution. Such a system can use a time variable field strength to tune the flipped wavelength to the central wavelength of a given time of flight.

Req. #	Parameter	Description	Value/Error
13.6.9.1r41	$\frac{\delta\lambda_{SSR}}{\lambda_{SSR}}$	Relative spatial-spin-resonance flipper wavelength resolution	1%

3.4.5 Neutron attenuation system

There shall be an automated attenuator changing system, far enough from the experimental cave to avoid background from neutrons scattering in the attenuators. The middle focus position seems most suitable for this application.

Req. #	Parameter	Description	Value/Error
13.6.9.1r42	ΔA	Attenuation factor range available	1-10 ⁵
13.6.9.1r43	N_{atten}	Minimum number of attenuation steps for the given range	4

3.5 Beam Validation System (13.6.9.1.6)

Beam and flux monitoring shall be available at different positions of the beamline. Especially the beam passing through the VS and middle focus positions need to be evaluable.

Req. #	Description
13.6.9.1r44	PSD monitor at middle focus for beam characterization, removable out of beam if feasible
13.6.9.1r45	High transmission ToF monitor behind beam collimation in front of sample for normalization purposes
13.6.9.1r46	Several simple flux monitors with high transmission at important points of the beamline

3.6 Flight Tube (13.6.9.1.7)

To reduce background and intensity loss from air scattering, as much of the neutron flight path before the sample shall be evacuated. Flight tubes need to be designed in conjunction with beamline shielding to avoid unwanted contamination of the neutron beam from fast neutrons.

3.7 Beam Cut Off (13.6.9.1.8)

There shall be a shutter system that can be closed for cave access and allow maintenance access to other instrument areas as much as reasonably achievable.

Req. #	Description
13.6.9.1r47	Shutter has to have enough beam attenuation to allow safe access to the experimental cave
13.6.9.1r48	A failsafe mechanism should be implemented
13.6.9.1r49	Most up-stream position for shutter is desired to have maintenance to other areas of the beamline during neutron production
13.6.9.1r50	PSS regulations need to be followed, e.g. beam monitor behind shutter to verify shutter closed state

3.8 Vacuum System (13.6.9.1.9)

As the *Estia* chopper system does not work with very high speeds the only necessary requirements for the beamline vacuum are to reduce neutron scattering and creation of activated gas. For these purposes a rough vacuum is already sufficient. The vacuum shall be divided into separable sectors, to allow maintenance at each Selene guide mirror,

the VS+Chopper and in the experimental cave region without breaking vacuum in the other sectors.

Req. #	Parameter	Description	Value/Error
13.6.9.1r51	V_{min}	Minimum necessary vacuum quality for the neutron guide system	1 mbar
13.6.9.1r52	V_{goal}	Desired vacuum quality for the neutron guide system	10^{-3} mbar
13.6.9.1r53	V_S	Minimum number of separable vacuum sectors	4

Req. #	Description
13.6.9.1r54	Vacuum windows should be avoided as much as possible to reduce scattering losses of the neutron beam

3.9 Shielding (13.6.9.1.10)

In general, the instrument shielding should minimize the background at the experimental cave and protect from harmful radiation doses. For the background reduction, a signal to background ration better then 10^7 is necessary.

Req. #	Parameter	Description	Value/Error
13.6.9.1r55	S/B	Minimum signal to background ratio to be achieved by instrument shielding.	10^7

3.9.1 In-Bunker Shielding (13.6.9.1.10.1)

The main purpose of the in-bunker shielding is to minimize the number of unused neutrons entering the bunker wall and with it the beamline. Special care needs to be taken to reduce high energy neutron background, that needs large amounts of material to be stopped. Additionally in-bunker shielding can be used to protect the VS motion control equipment to increase the system lifetime.

As with the heavy collimation outside the bunker, the in-bunker shielding should block direct sight through the Feeder as much as possible. In addition a collimation close to the VS position, where the beam size is smallest, is desirable.

Req. #	Parameter	Description	Value/Error
13.6.9.1r56	HC_1	Approximate position of first heavy collimation block to cut direct sight within the feeder.	3-5.5 m
13.6.9.1r57	HC_2	Approximate position of second heavy collimation block around the beam to reduce unused flux on and after the VS.	8-10.8 m
13.6.9.1r58	R_{VS}	Desired radiation dose rate at motion control components of virtual source	<1 Rad/h
13.6.9.1r59	HC_3	Approximate position of third heavy collimation block around the beam to reduce unused flux after the VS.	11.2-12 m

3.9.2 Beamline Shielding (13.6.9.1.10.1)

The biological beamline shielding shall fulfill the ESS safety requirements (*ESS-0001786* - $<3 \mu\text{Sv/h}$) at any given point outside the shielding wall. It begins at the outer radius of the bunker wall and ends at the experimental cave. Access to open the shielding shall be controlled with PSS equipment, so stacking of shielding to minimize PSS costs by reducing e.g. the number of keys to secure the plates need to be considered. If possible, the beamline shielding allow access to as much area of the beamline during neutron operation as feasible. The shape of the shielding plates shall prevent streaming paths for fast neutrons by using chicanes following the 10x rule (chicane offset at least 10x the opening size).

Req. #	Parameter	Description	Value/Error
13.6.9.1r60	R_{max}	Maximum allowed radiation dose rate outside the beamline shielding from MCNP simulations	$1 \mu\text{Sv/h}$
13.6.9.1r61	ΔC	Minimum chicane offset with respect to opening size to prevent streaming	10x
13.6.9.1r62	PSS	PSS control for opening of beamline shielding shall be available with cost optimized implementation	

3.9.3 Neutron Guide Shielding (Heavy Collimation) (13.6.9.1.10.1)

The shielding within the Selene guide system is necessary to break the direct line of sight for fast and thermal neutrons through the elliptical guides. In addition, the albedo transport through the beamline should be minimized. There are 7 optimal positions for heavy collimation within the Selene guide system. How many of these collimation sages need to be equipped with heavy shielding blocks needs to be decided with MCNP calculations to fulfill the S/B requirement.

Req. #	Parameter	Description	Value/Error
13.6.9.1r63	HC_{S1-1}	Approximate position of collimation block before Selene guide 1 to block beams outside the ellipses. Heavy collimation at this position has the additional benefit of shielding the Selene guide 1 components from high radiation doses.	13 m
13.6.9.1r64	HC_{S1-2}	Approximate position of collimation block within Selene guide 1 to block beams passing through the direct line between foci.	17 m
13.6.9.1r65	HC_{S1-3}	Approximate position of collimation block before Selene guide 1 to block beams outside the ellipses.	21 m
13.6.9.1r66	HC_{CF}	Approximate position of collimation block close to the central focus between Selene guides 1 and 2.	23 m
13.6.9.1r67	HC_{S2-1}	Approximate position of collimation block before Selene guide 2 to block beams outside the ellipses.	25 m
13.6.9.1r68	HC_{S2-2}	Approximate position of collimation block within Selene guide 2 to block beams passing through the direct line between foci.	29 m
13.6.9.1r69	HC_{S2-3}	Approximate position of collimation block before Selene guide 2 to block beams outside the ellipses. Heavy collimation at this position should be avoided, as it is already within the experimental cave.	30 m

4 Sample Exposure System (13.6.9.2)

4.1 Sample Positioning (13.6.9.2.1)

The sample positioning needs to allow the adjustment of the sample surface to the incident beam focus by correcting any possible sample miss-orientation on the sample holder and give access to all necessary incident beam angles. It shall accommodate the weight of the sample environment equipment and sample holders, in particular allowing to accommodate pool sample environment as necessary. The alignment precision of the different axes follows from the beam geometry and maximum instrument resolution. In particular the most precise axes are the Y-translation (parallel to sample surface normal) due to the small projected footprint of $60\ \mu\text{m}$ in this direction and the omega rotation, which needs to be matched to the angular instrument resolution.

Req. #	Parameter	Description	Value/Error
13.6.9.2r1	X_{range}	Horizontal translation parallel to sample surface (parallel to beam at $\omega = 0$)	$\pm 20\ \text{mm}$
13.6.9.2r2	δX	X translation accuracy	$50\ \mu\text{m}$
13.6.9.2r3	Y_{range}	Horizontal translation perpendicular to X (surface normal)	$\pm 5\ \text{mm}$
13.6.9.2r4	δY	Y translation accuracy	$2.5\ \mu\text{m}$
13.6.9.2r5	Z_{range}	Vertical translation	$\pm 20\ \text{mm}$
13.6.9.2r6	δZ	Z translation accuracy	$50\ \mu\text{m}$
13.6.9.2r7	ω_{range}	Rotation range around Z-axis (incident beam angle)	$-10^\circ - +90^\circ$
13.6.9.2r8	$\delta\omega$	Rotation accuracy for ω	0.0025°
13.6.9.2r9	χ_{range}	Rotation range around X-axis (incident beam angle)	$\pm 5^\circ$
13.6.9.2r10	$\delta\chi$	Rotation accuracy for χ	0.05°

The sample area shall have enough flexibility to allow ESS pool sample environment (see *ESS-0038078*) and user supplied equipment to be installed. An example would be an in-situ film deposition chamber, a heavy vacuum vessel with large footprint. For this purpose a second sample platform might be desirable.

Req. #	Parameter	Description	Value/Error
13.6.9.2r11	A_{SE}	Minimum available area around the sample position to be accessible for bulky sample environment	1.0x1.5 m ²
13.6.9.2r12	A_{AX}	Additional area within the experimental cave to be available for SE auxiliary equipment (within 2 m of sample position)	up to 4 areas 2 m ² total
13.6.9.2r13	m_{SE-I}	Required weight to be installable on the default sample positioning stage	300kg
13.6.9.2r14	m_{SE-P}	Required weight for pool SE to be accommodated	1000kg
13.6.9.2r15		Sample stage should follow motion control standards from ESS (<i>ESS-0037290</i>)	

4.2 Sample Environment Equipment (13.6.9.2.3)

In addition to being able to accommodate electric field and cryomagnet equipment from the ESS sample environment (SE) pool the large expected demand for low temperatures and magnetic fields necessitates instrument specific sample environment. For in-situ annealing experiments a high temperature option would be desirable. Additionally, the sample environment for reflectometry experiments should have the least amount of material in the beam to minimize background from scattering of these materials.

As measurements with very small counting times can be anticipated in the high intensity mode, a quick exchange of samples is very important to minimize loss of beamtime. Sufficient number of sample holders with 5x5 mm² to 20x20 mm² attachment plates should be provided, including a quick exchange mechanism. Fast cooling equipment and optimized room temperature sample holders/changer will improve the throughput considerably.

Liquid handling equipment compatible with ones used at FREIA should be provided as instrument specific SE, too.

Req. #	Parameter	Description	Value/Error
13.6.9.2r16	S_{sample}	Minimum available sample space for any SE equipment.	20x20 mm ²
13.6.9.2r17	T_{range}	Default available temperature range for instrument specific SE	5K - 300K
13.6.9.2r18	$T_{HT-range}$	Optional temperature range for annealing experiments	300K - 700K
13.6.9.2r19	H_{range}	Minimum homogeneous in-plane field available at the sample position provided by instrument specific SE	±1T
13.6.9.2r20	E_{range}	Electric field provided from pool SE	±10kV
13.6.9.2r21	t_{SC-max}	Maximum average time between measurements of different samples at base temperature	30 min

Req. #	Description
13.6.9.2r22	The amount of material in the beam shall be minimized for the instrument specific SE
13.6.9.2r23	A room temperature vacuum sample holder and sample changer should be provided
13.6.9.2r24	Sufficient number of sample holders with 5x5 mm ² up to 20x20 mm ²
13.6.9.2r25	Liquid handling equipment compatible with FREIA

4.3 Non-Sample Environment Ancillary Equipment (13.6.9.2.4)

To improve and accelerate the sample alignment procedure a optical alignment system shall be available. If feasible, this system should implement a neutron beam independent automatic alignment procedure for the compensation of Y and ω misalignment even within the low temperature sample setup.

Req. #	Description
13.6.9.2r26	An optical alignment support shall be installed
13.6.9.2r27	Automatic (re-)alignment with the optical system should be implemented.

5 Scattering Characterization System (13.6.9.3)

5.1 Polarization analyzer system (13.6.9.3.1)

The considerations for the analyzer are equal to that of the polarizers explained in section 3.4.2, with the exception that it does not need to cut frame overlap neutrons and that it can only be positioned on the detector arm after the sample. Therefore the two subsequent transmission mirrors should use different angles of incidence to be stacked after each other, which necessitates different m-values for the first and second mirror. For off-specular scattering experiments the analyzer shall not only cover the 1.5° high intensity beam divergence but up to at least 4° of total divergence. The ability to measure both the reflected and transmitted beam of a vertically curved analyzer has the huge advantage to reduce measurement time by a factor of 2 and to allow single pulse measurements of both spin states. As vertical curvature will limit the performance of the device due to the larger beam size in vertical direction, an operation of the analyzer with 90° rotation should be implemented.

Req. #	Parameter	Description	Value/Error
13.6.9.3r1	$\Delta\Theta$	Scattering angle covered by analyzer setup (horizontal and vertical)	$\pm 2^\circ$
13.6.9.3r2	$m_{Analyzer1}$	Supermirror coating for the transmission polarizers (Fe/Si)	4
13.6.9.3r3	$m_{Analyzer2}$	Supermirror coating for the transmission polarizers (Fe/Si)	5

Req. #	Description
13.6.9.3r4	Multiple mirror segments that distort the scattered beam shall be avoided
13.6.9.3r5	Analyzer should allow vertical operation, capturing reflected and transmitted beams with the detector
13.6.9.3r6	Analyzer should allow horizontal operation, to achieve higher polarization efficiencies

5.2 Neutron detector system (13.6.9.3.2)

Two separate detectors, one for each of the vertical beams, shall be provided (one initial and one after upgrade to two guides). The detectors shall be able to capture the full vertical divergence of the beam and reflection from the analyzer as well as off-specular scattering. The resolution needs to be sufficient to achieve comparable $\delta\Theta/\Theta$ resolution at small incident angles to the wavelength resolution $\delta\lambda/\lambda$ for the application of the high intensity mode. As reference samples with supermirror coating will be measured for normalization purposes, the count rate capability must be outstanding. It is expected that the maximum count rate density found for this purpose (or close to the critical edge for normal samples) in simulations (4 MHz/mm²) is not achievable, therefore the highest achievable rate together with an automated attenuation system (see section 3.3.2) needs to be provided.

Req. #	Parameter	Description	Value/Error
13.6.9.3r7	L_D	Distance sample to detector	4 m
13.6.9.3r8	$2\Theta_{range}$	Rotation range around Z-axis for reflectometry to reach 1\AA^{-1} at 8\AA (scattered beam angle)	$-10^\circ - +80^\circ$
13.6.9.3r8.1	$2\Theta_{diff}$	Desired rotation angle around Z-axis for diffraction	$+135^\circ$
13.6.9.3r9	$\delta 2\Theta$	Rotation accuracy for 2Θ	0.005°
13.6.9.3r10	δX	Horizontal detector resolution	0.5 mm
13.6.9.3r11	δZ	Vertical detector resolution	4 mm
13.6.9.3r12	D_X	Horizontal detector size	500 mm
13.6.9.3r13	D_Z	Vertical detector size	250 mm
13.6.9.3r14	f_{CR}	Maximum expected count rate	4 MHz/mm ²
13.6.9.3r15	δt_{ToF}	Detector time resolution	1 ms
13.6.9.3r16	$\epsilon_{4\text{\AA}}$	Detector efficiency at 4\AA	45%
13.6.9.3r17	ϵ_γ	Detector sensitivity to gamma radiation	10^{-6}

Req. #	Description
13.6.9.3r18	Intensity cross-talk between horizontal pixels should be minimized. This includes reduction of entrance windows thickness to a minimum.
13.6.9.3r19	The detector vessel shall be shielded from all sides against neutron background from other directions by absorbing plates.

In the high intensity focusing reflectometry mode the detector together with the wavelength resolution limit the available q_z resolution ($\delta q_z/q_z = \sqrt{(\delta\Theta/\Theta)^2 + (\delta\lambda/\lambda)^2}$). While improving wavelength resolution always reduces intensity the increase in detector to sample distance or pixel resolution, although having other design implications, keep the measured intensity constant. To make sure the detector resolution does not reduce the measured q_z resolution in the main bandwidth (4\AA - 11\AA for most experiments) at small angles (0.8°) the detector resolution should be $\approx 3x$ better than the wavelength resolution (as $\sqrt{1/9 + 1} \approx 1$). The natural wavelength resolution for *Estia* is $\delta\lambda=0.3\text{\AA}$,

thus for the 11\AA neutrons that measure the small q_z values close to the critical edge a $\delta\Theta/\Theta \approx 1\%$ would be desirable. In addition the optional high resolution mode proposed as upgrade will deliver $\delta\lambda/\lambda \approx 1\%$ and would not improve the q_z resolution at the critical edge region if the detector resolution wasn't matched to this value. In both cases the necessary angular resolution of 0.008° can be achieved using 0.5 mm detector resolution at 4 m distance from the sample.

5.3 Flight tube system (13.6.9.3.4)

The beam path after the sample shall be equipped with a flight tube to reduce air-scattering background and shield the detector against neutrons not originating from the sample position. The tube can be either argon filled or evacuated but should be able to get as close to the sample as possible and accommodate the polarization analyzer and spin-flipper.

Req. #	Description
13.6.9.3r20	The flight tube shall cover most of the distance after the sample up to the detector
13.6.9.3r21	The flight tube shall be clad with neutron absorbing material
13.6.9.3r22	The flight tube sides shall avoid possible indirect paths from areas around the sample to the detector to reduce possible background (e.g. reflection from the tube sides)

6 Optical Cave (13.6.9.4)

There is no area perceived for *Estia* that would be considered an optical cave, therefore there are no requirements given here.

However, a decision might be made at a later stage to redefine components that are downstream from the instrument shutter to be categorized a optical cave. This could be all components between the end of Selen guide 1 and the entrance into experimental cave, i.g. the middle focus components, polarizer optics and Selene guide 2. Access to these components during normal beam operation and without opening the biological shielding might have advantages.

7 Experimental Cave (13.6.9.5)

7.1 Personal Safety System (13.6.9.5.1)

The experimental cave shall be equipped with an access control system following the safety standards provided by the ESS PSS group. Part of the system will be a radiation safe entrance door with chicane, oxygen deficiency warning system and electrical, shutter and motion control emergency switches. Necessary vacuum, cryogenic liquids and magnetic field safety measure shall be taken within ESS safety regulations. (For some of these regulations see *ESS-0002381*, *ESS-0034035* and *ESS-0001786*.)

Req. #	Description
13.6.9.5r1	PSS follows ESS regulations not yet defined
13.6.9.5r2	Cave access only possible when beam shutter is known to be closed and no radiation is measured behind the shutter

7.2 Utilities distribution and support infrastructure (13.6.9.5.2 and 13.6.9.5.3)

The necessary utilities and infrastructure follow from the equipment placed within the Experimental cave.

7.2.1 Remote viewing (13.6.9.5.3.9)

To monitor instrument motion during remote control from the hutch, a network camera shall be installed within the experimental cave. Depending on Swedish work regulations this camera might need an interlock to shut down during user access to the cave.

7.3 Shielding (13.6.9.5.4)

The cave shielding shall at any circumstance limit the dose rate outside the walls below ESS limitations. Streaming paths will be avoided as described in section 3.9.2. Skyshine

and groundshine contributions, as far as estimated by the ESS shielding group, shall be reduced to not impact the signal to background ratio.

Req. #	Parameter	Description	Value/Error
13.6.9.5r3	R_{max}	Maximum allowed radiation dose rate outside the cave shielding	1 μ Sv/h
13.6.9.5r4	ΔC	Minimum chicane offset with respect to opening size to prevent streaming	10x
13.6.9.5r5	S/B	Minimum signal to background ratio to be achieved by cave shielding.	10^7

7.4 Cave structure (13.6.9.5.5)

The cave structure must be able to cope with the weight of the ceiling necessary for the shielding against skyshine. Cave height shall be sufficient to install pool SE and the floor footprint shall allow the full detector arm rotation and enough space for additional electronic and SE equipment. Top side access to the cave with an instrument specific crane is necessary.

Req. #	Description
13.6.9.5r6	Ceiling shall accommodate shielding weight
13.6.9.5r7	Top side access for crane
13.6.9.5r8	A local crane with 2T maximum load shall be provided for the instrument, which allows to bring materials and SE equipment from outside the cave through the roof to the sample position
13.6.9.5r9	Large enough footprint for detector rotation and additional SE and electronic equipment
13.6.9.5r10	Considerations for high magnetic fields as described in <i>ESS-0038078</i> shall be taken to accommodate level 3 SE
13.6.9.5r11	A dedicated storage cabinet for SE equipment shall be provided
13.6.9.5r12	Tools shall be available within the cave

7.5 Sample environment control box (13.6.9.5.6)

The cave shall have a fixed installed control box for all supplies necessary to operate the SE equipment (*ESS-0038163*).

Req. #	Description
13.6.9.5r13	Provide SE power
13.6.9.5r14	Provide supply gases (N2, Ar, LHe)
13.6.9.5r15	Provide chilled water
13.6.9.5r16	Provide compressed air

7.6 Instrument control terminal

To be able to quickly move instrument hardware as the detector arm from within the cave, there shall be a separate computer terminal to allow access to the motion control system.

Req. #	Description
13.6.9.5r17	An instrument control terminal for operating the beamline shall be present in the hutch

8 Control Hutch (13.6.9.6)

Experiments will be controlled remotely from within an enclosed control hutch. The hutch needs to provide ample space to coordinate the experiments and perform initial data analysis for one full experimental team (users plus beamline personal). For short amounts of time an overlap of two experimental teams will be probable and shall be considered in the layout procedure. Enough computing infrastructure needs to be provided within this area to perform the mentioned tasks.

8.1 Support infrastructure (13.6.9.6.1)

The necessary utilities and infrastructure follow from the equipment placed within the control hutch.

8.2 Hutch building (13.6.9.6.2)

Req. #	Description
13.6.9.6r1	The hutch building shall be sufficiently sized for multiple user operation
13.6.9.6r2	Electronic equipment shall be shielded against interference from the instrumental hall

8.3 Computer access

Req. #	Description
13.6.9.6r3	An instrument control terminal for remotely operating the beamline shall be present in the hutch
13.6.9.6r4	Two data reduction and analysis terminals, separate from the control terminal, shall be present

9 Sample Preparation Area (13.6.9.7)

9.1 Utilities distribution and support infrastructure (13.6.9.7.1 and 13.6.9.7.2)

The necessary utilities and infrastructure follow from the equipment placed within the Experimental cave.

9.2 Cabin building structure (13.6.9.7.3)

Depending of the location for the sample preparation area it can be either enclosed in a similar manner as the control hutch or consist only of a dedicated working area without separate enclosing.

9.3 Laboratory equipment and sample storage (13.6.9.7.4)

The sample area needs to be supplied sufficiently to allow efficient preparation of the samples for the experiments as well as storage for irradiated samples. This leads to the following minimal equipment requirements:

Req. #	Description
13.6.9.7r1	Provide radiation safe sample storage cabinet
13.6.9.7r2	Provide cleaning solvents (ethanol, propanole, acetone, DI-water)
13.6.9.7r3	Provide dust and moisture removal with clean pressurized air or N ₂
13.6.9.7r4	Provide sample handling (tweezers)
13.6.9.7r5	Provide means to attach samples to holders (vacuum grease, sliver paint)
13.6.9.7r6	Provide sample holder stand for convenient installation of samples

Req. #	Description
13.6.9.7r7	Optical sample pre-alignment stage is desirable
13.6.9.7r8	Standard tool box for SE equipment etc. shall be provided
13.6.9.7r9	A sufficiently sized workbench with chemical and heat resistant surface shall be provided
13.6.9.7r10	Magnifying glass lamp and small microscope for sample manipulation will be necessary
13.6.9.7r11	Safe mounting points for removable SE equipment shall be provided
13.6.9.7r12	A set of reference samples (sample sized supermirrors, multilayers and standard films)

10 Utilities Distribution (13.6.9.8) and Support Infrastructure (13.6.9.9)

As *Estia* is placed in Hall 1 solely, all components of the instrument will have to be connected to the Hall 1 utilities distribution system. The necessary requirements follow from the equipment distribution within the instrumental hall.

11 Control Racks Hall 1 (13.6.9.10.1)

11.1 DAQ (13.6.9.10.1.1)

The data acquisition control hardware needs to be well grounded and shielded against electronic noise. *Estia* will follow the ESS detector group guidelines in this respect (*ESS-0051373*).

11.2 DMSC (13.6.9.10.1.2)

All necessary interfaces to access DMSC infrastructure has to be provided. This will require coordination between DAQ, DMSC, choppers, vacuum, PSS, SE and motion control to fully integrate the different beamline components.

11.3 Motion control (13.6.9.10.1.3)

As there will be several motion control units distributed over a large area of the instrument, it is expected that a separation into different motion control racks is advantageous. The position of the racks, however, shall be chosen to allow access during beam operation with open shutters.

Req. #	Description
13.6.9.10.1r1	Separate control racks for distributed motion units
13.6.9.10.1r2	Allow access during normal beam operation
13.6.9.10.1r3	Equipment should follow <i>ESS-0037290</i> for compatibility if possible

11.4 Chopper control (13.6.9.10.1.4)

The instrument will use the standard chopper control rack components defined by the ESS chopper group. Good access to the rack is desirable.

11.5 Vacuum control (13.6.9.10.1.5)

The instrument will use the standard vacuum control rack components defined by the ESS vacuum group. Good access to the rack is desirable.

11.6 PSS (13.6.9.10.1.6)

The instrument will use the standard PSS control rack components defined by the ESS PSS group.

11.7 Magnet control (13.6.9.10.1.7)

The instrument specific sample environment magnet will need a dedicated controller that has to allow access to the full magnetic field range, be easily accessible and compatible with the ESS SE control software (*ESS-0038165*).

Req. #	Description
13.6.9.10.1r4	The magnet controller shall allow full field range from negative to positive saturation of the magnets capabilities
13.6.9.10.1r5	Controller needs to comply with ESS standards
13.6.9.10.1r6	Easy access from outside the experimental cave is desirable

12 Integrated Control and Monitoring (13.6.9.11)

The integration with DMSC, PSS and other ESS defined systems shall be possible. *Estia* design will therefore need to follow the guidelines provided by the specific ESS and DMSC groups or consult these groups for approval of custom choices.

Estia has two specific integration tasks that might be outside the standard scope:

Req. #	Description
13.6.9.11r1	The optical alignment system at the sample position needs to be coupled to sample positioning motion, if necessary for specific experiments
13.6.9.11r2	Measurement and alignment of mirror segments need to be integrated in one software framework

Bibliography

- [1] J. Stahn, U. Filges, and T. Panzner. Focusing specular neutron reflectometry for small samples. *Eur. Phys. J. Appl. Phys.*, 58(1):11001, 2012.
- [2] J. Stahn and A. Glavic. Focusing neutron reflectometry: Implementation and experience on the tof-reflectometer Amor. *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment*, 821:44–54, June 2016.

Referenced ESS Documents

- ESS-0001786** Definition of Supervised and Controlled Radiation Areas
- ESS-0002381** ESS Fire Protection
- ESS-0034035** Selection of electrical cables with respect to Fire Safety
- ESS-0037290** Motion Control Components Standard for ESS Applications
- ESS-0038078** ESS Sample Environment Mechanical Interfaces for Instruments
- ESS-0038163** ESS Sample Environment Utility Supplies Reference Document
- ESS-0038165** ESS Sample Environment Control System Reference
- ESS-0051373** ESS Guidelines for Instrument Power and Grounding