



New Instrumentation for Large Scale Structures

Maximising the Scientific Impact of ESS

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<https://ess.eu/instrument-roadmap>

Call for Input to the ESS Instrument Roadmap

Call open until end of Jan 2026



ESS is pleased to invite the European scientific community to contribute input to a roadmap for instruments beyond the 15 currently under construction. This roadmap will guide future developments of the instrument suite, ensuring that ESS supports a versatile science portfolio in the decades to come. The call will be open for one year.

- We are looking for science driven proposals that suit the unique properties of neutrons and the possibilities offered by the high flux and flexible resolution of ESS
- The call is not limited to neutron scattering instruments but includes any scientific use of the neutron source.
- Need to leverage capacity and capability
- Need to leverage fundamental studies and innovation
- Encourage involvement of the community
- Engage in the process academia as well as ESS advisory committees

Contact us : instrumentroadmap@ess.eu

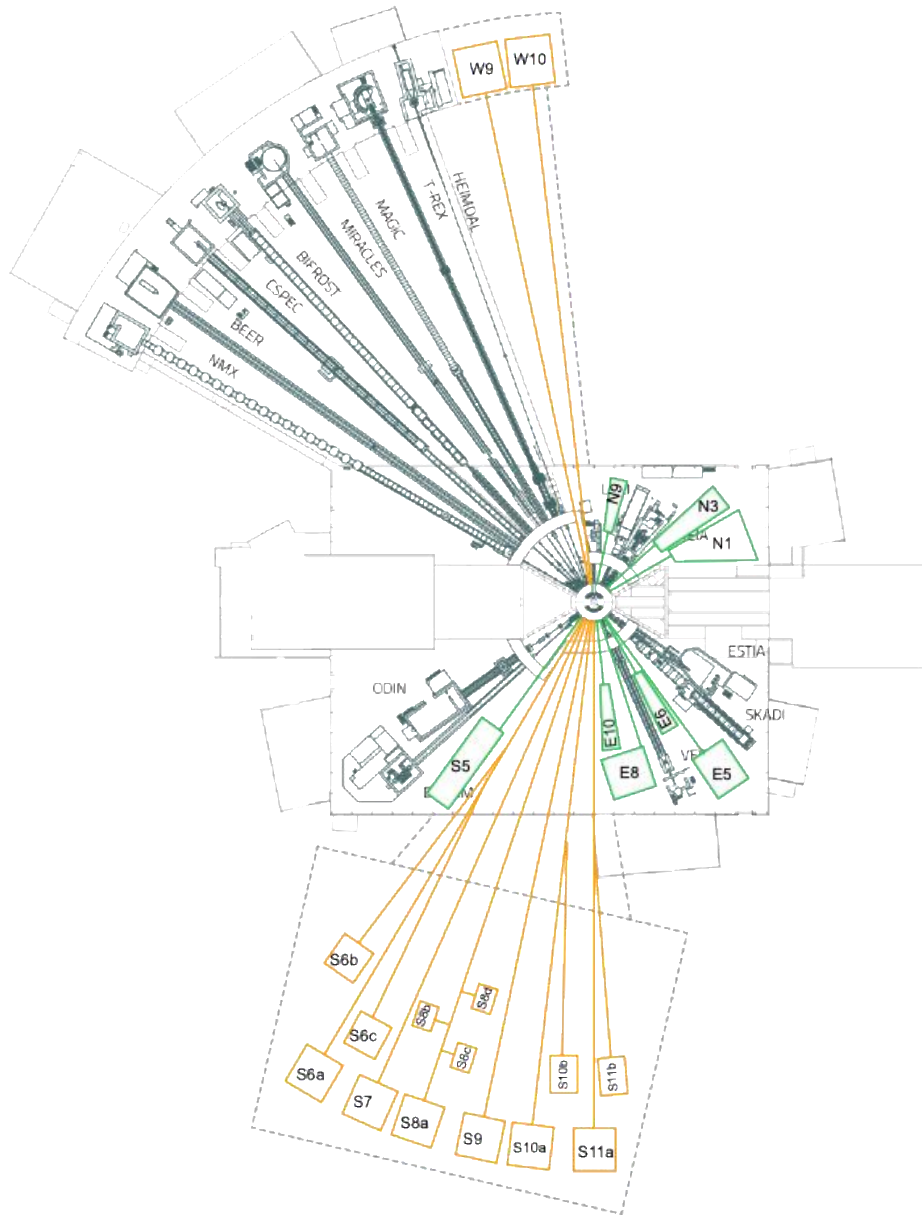
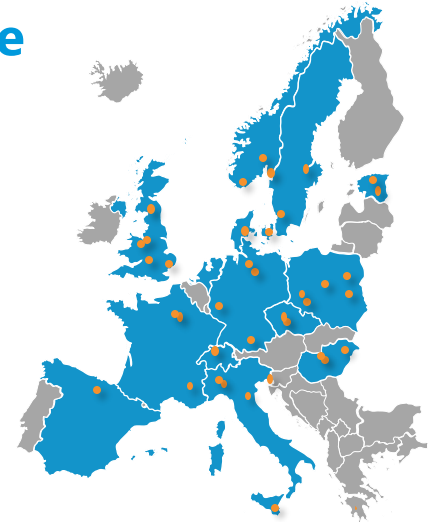


Interested parties in ESS member countries are welcome to submit proposals via our instrument divisions.

We aim at proposals supported by consortia of academic and research institutions including large involvement of ESS staff.

We plan to go beyond the in-kind model used so far and lead construction from the ESS.

We will strive to profit from the expertise of our European partners and we are looking now at possible collaboration models within a new **FRAMEWORK for PARTNERSHIPS (to be validated).**



Possible beamline positions fitting in existing experimental halls

Possible beamline positions requiring new or expanded experimental halls

Schematic of Possible Instrument Suite Expansion

Andrew Jackson 2024-10-16

Science Themes for New Instruments



Integrated Structural Biology and Biophysics

Bringing together multiple neutron techniques with computational methods and complementary techniques to answer complex structural biology and biophysics questions.

Formulations and Food

Complex multi-component systems require large parameter space studies with high throughput.

Geology and Geomaterials

Connecting with imaging and microscopy length scales to enable the study of structures from nanometres to millimetres

Surfaces and Interfaces

In-situ and in-operando 3D structural analysis of surfaces and interfaces

Industrial Usage

Lessons from nSOFT

nSoft Consortium

Non-proprietary environment where soft materials manufacturers gain expertise, drive innovation in neutron measurements.

nist.gov/nsoft

NIST

3M

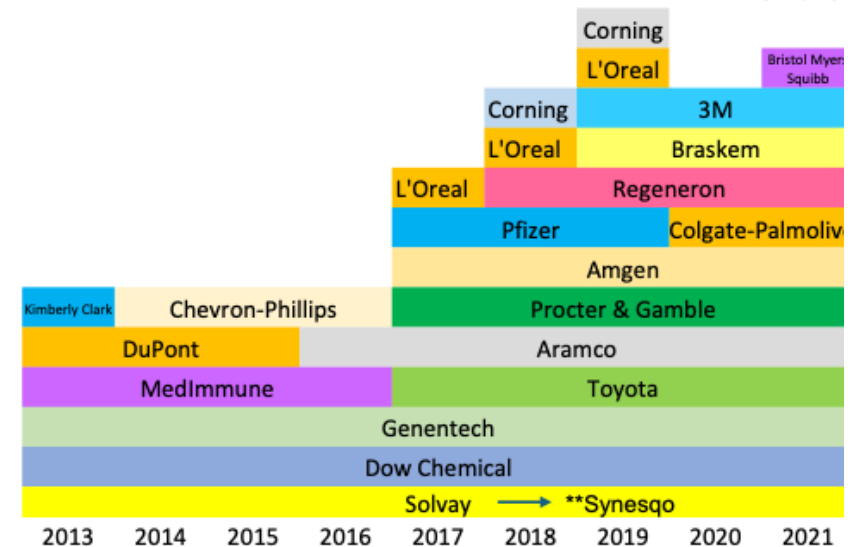
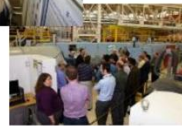
Dow

P&G

TOYOTA

Genentech
A Member of the Roche Group

SYENSQO



NIST nSOFT Consortium connects companies with neutrons via collaborative non-proprietary research projects.

Keys to success:

- Dedicated staff
- Dedicated, rapid access to beamtime

ESS has had a lot of interest from potential industrial users of SANS, reflectometry, and MX e.g.

- Tetrapak
- Alfa Laval
- Astra Zeneca
- Novo Nordisk

Large Scale Structures

Expanding ESS Experimental Capabilities

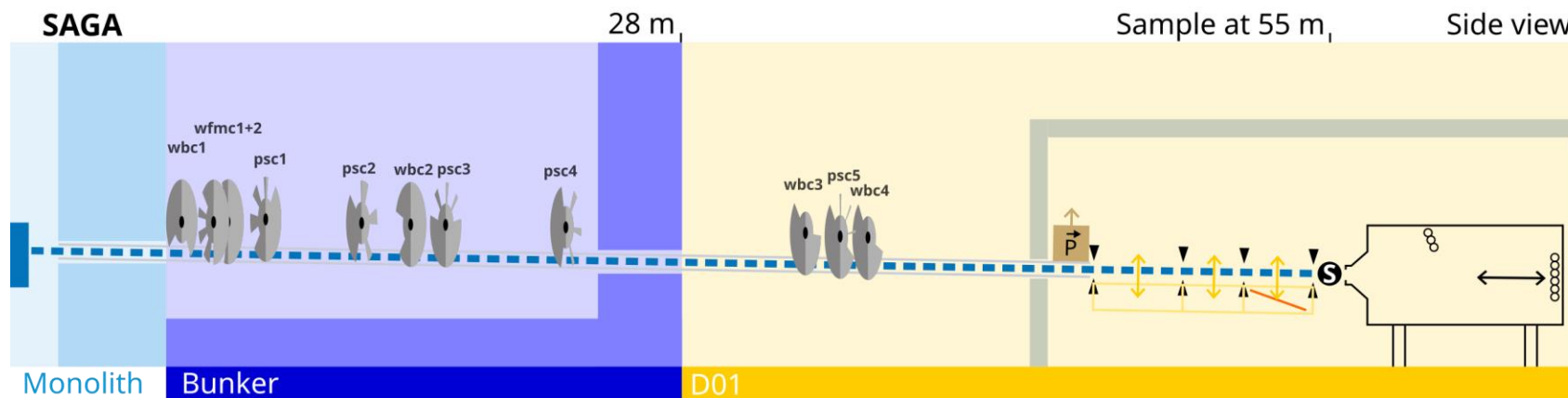
- **SAGA** – Dedicated surface scattering instrument for 3D studies of interfaces
- **Structural Biology Cluster** – 2nd NMX with DNP and a dedicated Bio-SEC-SANS
- **SMÅ** - High throughput SANS for industry and parametric studies*
- **ULL** – Membrane/Partially Ordered Systems Diffractometer*
- **MIMER** - Solid-Liquid Bio-Reflectometer*
- **Estib** – Small sample footprint reflectometer*
- **Yggdrasil** – Polarised SANS/WANS
- **SANS at very low Q** – VSANS/SEMSANS/USANS

Build on existing suite by providing new capabilities and increasing capacity to enable more complex experiments

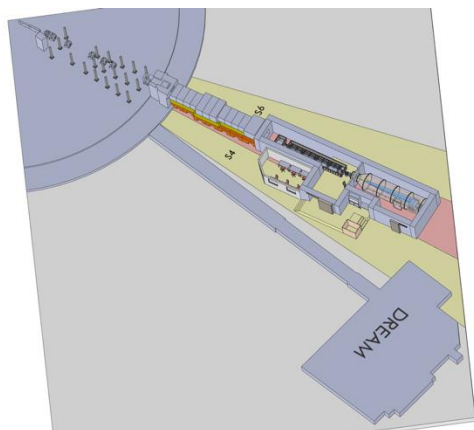
*names are preliminary and for convenience/entertainment only!

SAGA

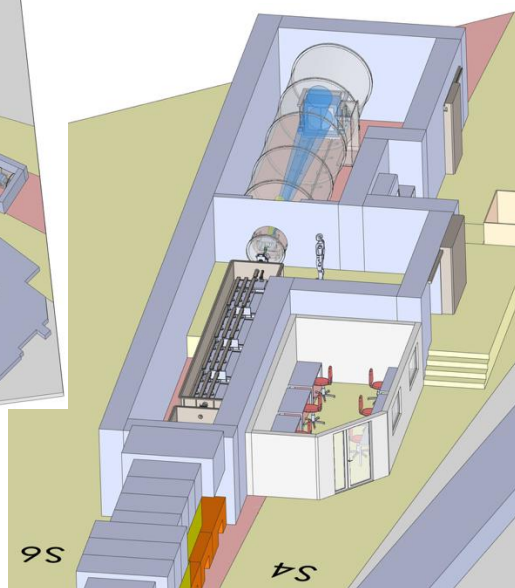
3D structural analysis of thin films and interfaces



SAGA – Quick facts	
Instrument length (GISANS/NR)	65m/58m
Bandwidth GISANS	3.7Å
λ-resolution for GISANS	2.1-4.4%
Bandwidth NR	4.2Å
λ-resolution for NR	2.3-4.9%
λ-resolution in WFM mode (both)	1%



Proposed location:
Beampoint S5 (next
to DREAM)



Science Case

- Energy & Materials
 - Organic photovoltaics and batteries
 - Advanced coatings
 - High speed measurements of structural changes during processing
- Quantum Materials
 - Magnetic thin films
 - Topological
 - Spintronics
- Life sciences & Soft Matter
 - Self-assembled structures
 - Model membranes / RAFTs

Technical features

- GISANS + NR on same sample
- TOF-GISANS => depth sensitivity
- Horizontal Surface => liquids
- Polarisation Analysis => magnetism
- π -GISANS type mode for higher flux => kinetics without depth sensitivity
- Possible k-focussing mode
- Capable of NR-Tomography
- Capable of transmission SANS

Structural Biology Cluster

Split beam extraction with two guides:

Protein diffractometer for dynamic nuclear polarisation

Expand protein crystallography availability and capability, building on the experience from NMX.

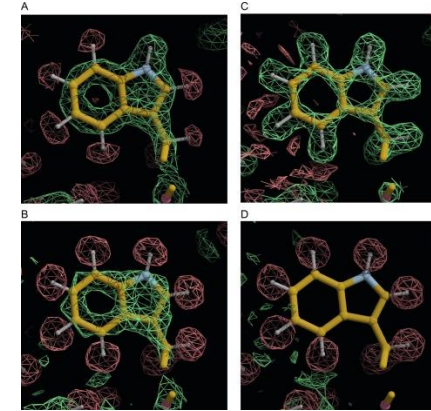
Non-magnetic end-station enabling DNP for background suppression

SANS/WANS end-station designed to study changes in protein structure in solution.

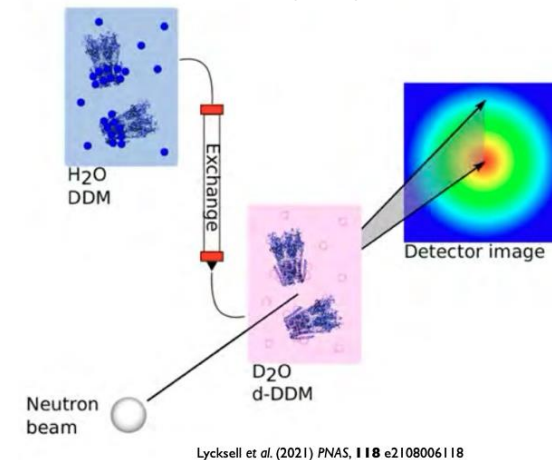
Q-range and resolution optimised for protein-in-solution and membrane protein-in-nanodisc studies.

Permanent SEC setup

Beamport S6



Pierce et al. (2020) *MIE*, **634**,153-175



Together with MaxIV, LU, and SciLifeLab we would be able to provide critical tools to the integrative structural biology toolbox.

SMA

High Throughput SANS

SMA : Studying Materials Automatically

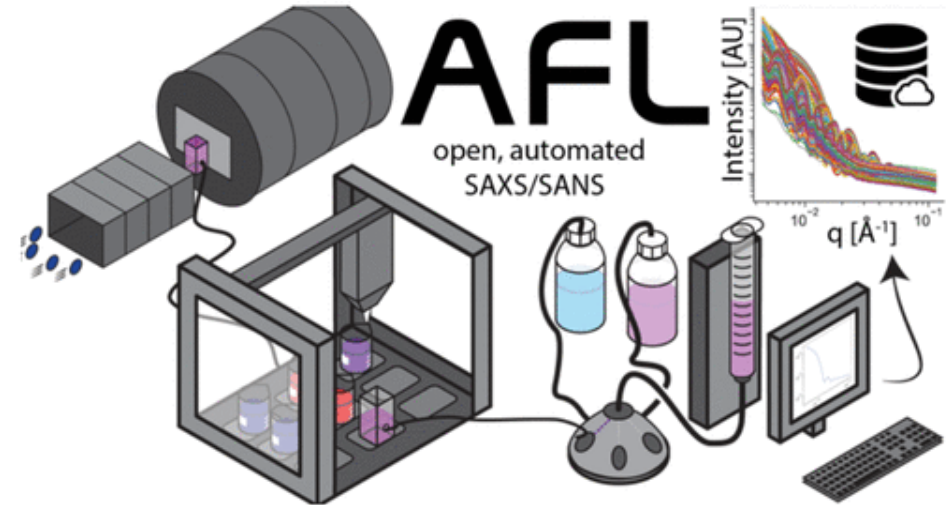
Science focus on large parametric studies of soft matter, complex fluids, and formulations.

Designed with the aim of efficiently supporting industrial measurements, rapid access, and mail-in.

Simple, fixed collimation SANS, with the option of different high throughput sample environments:

- Robotic autosampler
- Flow cell setup
- Automated/autonomous formulation using Machine Learning and physics-informed AI models

Beamport N9, N3, or E10 – or part of IDUN cluster



Chem. Mater. 2023, 35, 3, 846–852

<https://www.nist.gov/ncnr/ncnr-facility-upgrades/autonomous-formulation-lab-afl>

Yggdrasil

Polarised SANS/WANS



Marion Grzelka, Ioanna Chazapi, Gergory Chaboussant, Alexis Chennevière

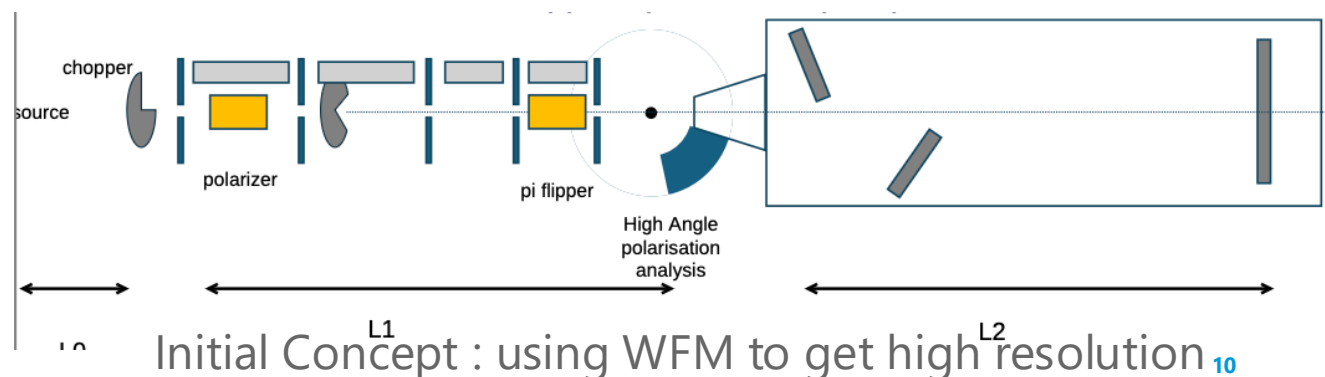
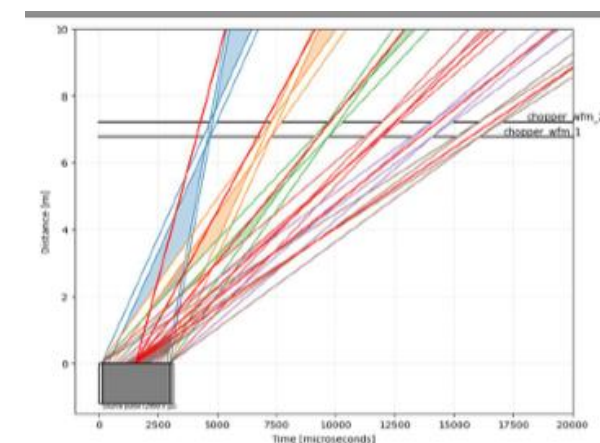
Extending SANS to High Q ($>5\text{\AA}^{-1}$) with polarisation analysis.

Increased capacity (SANS) with extended capability (WANS).

Connecting with DREAM Q range

Key Science Areas:

- Understanding hybrid inorganic-organic nanoparticles
- Polymer systems and composite materials
- Energy storage
- Porous materials
- Electrolytes



Membrane / Partially Ordered Systems Diffractometer

ULL : Understanding Lipids and Liquids

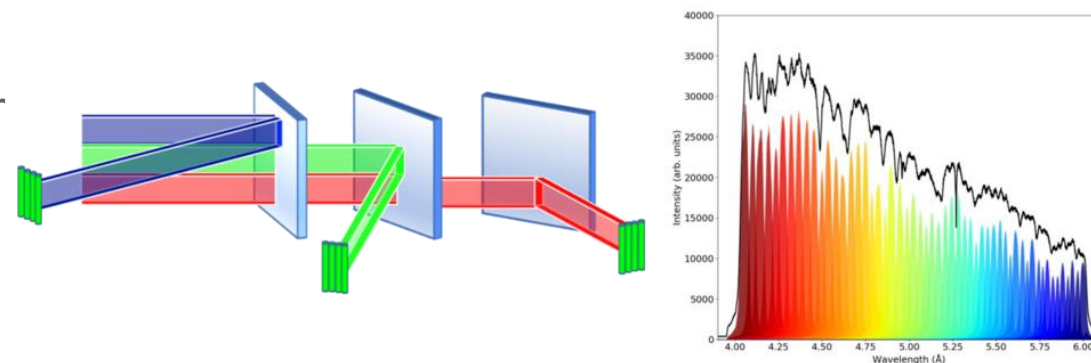
Instrument for membrane diffraction and WANS (for example liquid crystals, polymer crystallinity)

Investigating the possibility of also doing “liquids” diffraction – e.g. structuring of solvents around macromolecules or macromolecular assemblies.

Various technical solutions possible, but we are considering CANDOR type backend (multi-analyser energy selection) to obtain required wavelength resolution

Beamport N3, E10, or S6 (shared with structural biology cluster)

- Candor has 2Å bandwidth with Q resolution, dQ/Q , ~2.5%
- Low-background - 8 orders of magnitude dynamic range – ideal for low scattering applications
- Suitable for wide angle detector geometries



Credit: Brian Kirby and David Hoogerheide (Left) Schematic illustrating the wavelength selection of pyrolytic graphite monochromators (right) measured wavelength sensitivity associated with each individual detector for an example CANDOR array. Solid black line is the summed intensity vs. wavelength.

MIMER

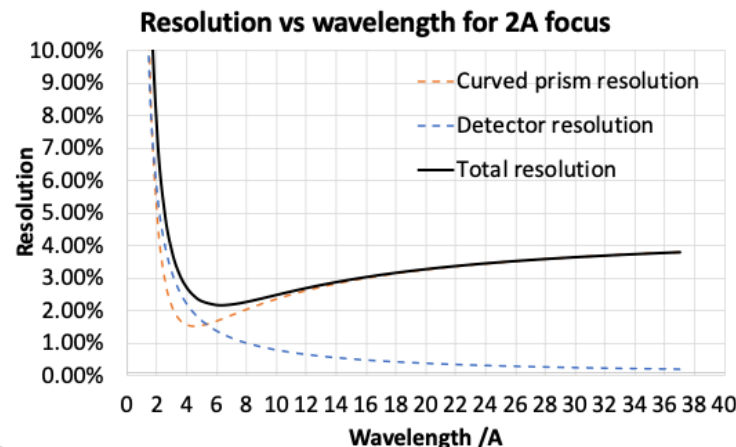
Solid-Liquid Bio-Reflectometer

MIMER : Measuring Interfaces and Membranes at ESS with Reflectometry

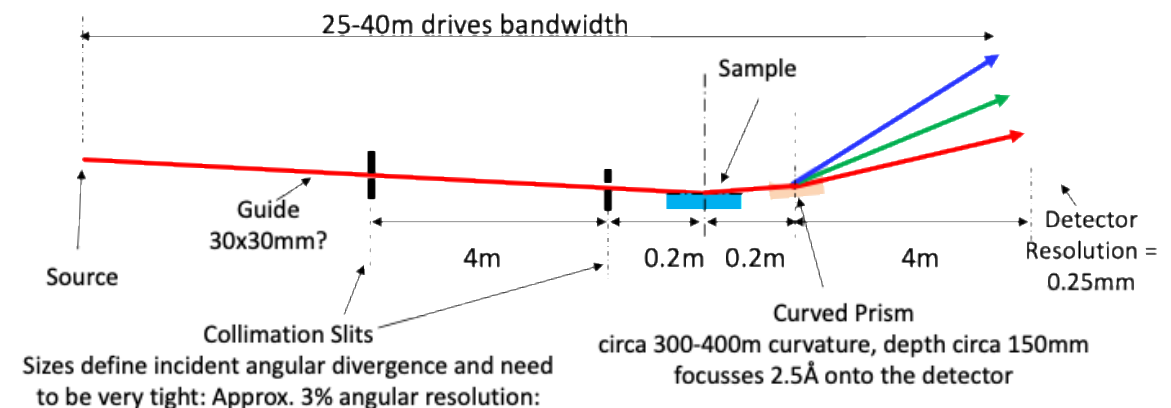
Expanding ESS capabilities for the support of studies of lipid membranes and protein-membrane interactions.

Estia and FREIA will be able to support these studies, but this instrument increases capacity and is optimised for work-horse solid-liquid experiments.

Beamport N3 or
Split guide



- Short instrument to provide wide bandwidth
- No complex chopper system – resolution is delivered by RAINBOWS or CANDOR in the end station
 - Rainbows can deliver resolution <4% using modified multiblade concept.
 - CANDOR can potentially remove inelastic scattering to improve background
- Optimised for high-throughput of solid-liquid samples
 - Includes substantial effort on automation (sample changing, intelligent decision making)
- Include polarisation for magnetic reference layers
- Limited to samples without off-specular scattering
- Sample space may be restricted by optics



Estib

Small Sample Footprint Reflectometer



Duplicate of Estia

- Leverage experience of Estia construction
- Drive down sample volume for biological experiments and improve signal to background
- Enable more complex experiments by increasing availability of small footprint reflectometry beamtime
- Focus on optimisation for electrochemistry and in-situ surface modification experiments, and use of environmental chambers and shear cells.



SANS at very low Q

VSANS/SEMSANS/USANS

Science Areas:

- GUV/Lipids
- Protein aggregation
- Polymer composites
- Geology
- Nano to microparticles and interactions

Connect to Imaging size range

Complementary to neutron grating interferometry on ODIN

Multiple Instrumentation Ideas:

- Compact pinhole VSANS (reduced complexity, ISIS currently in the process of developing this) – upgrade to SKADI alongside slit VSANS
- SEMSANS – possible upgrade to SKADI or dedicated SANS/SEMSANS instrument, could be combined with Yggdrasil proposal
- DCD USANS (Bonse-Hart) – making use of high integrated flux of ESS to deliver world leading USANS capability

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