Overview of GISANS initiative for ESS

SAGA – A Swedish Initiative for a GISANS instrument at ESS

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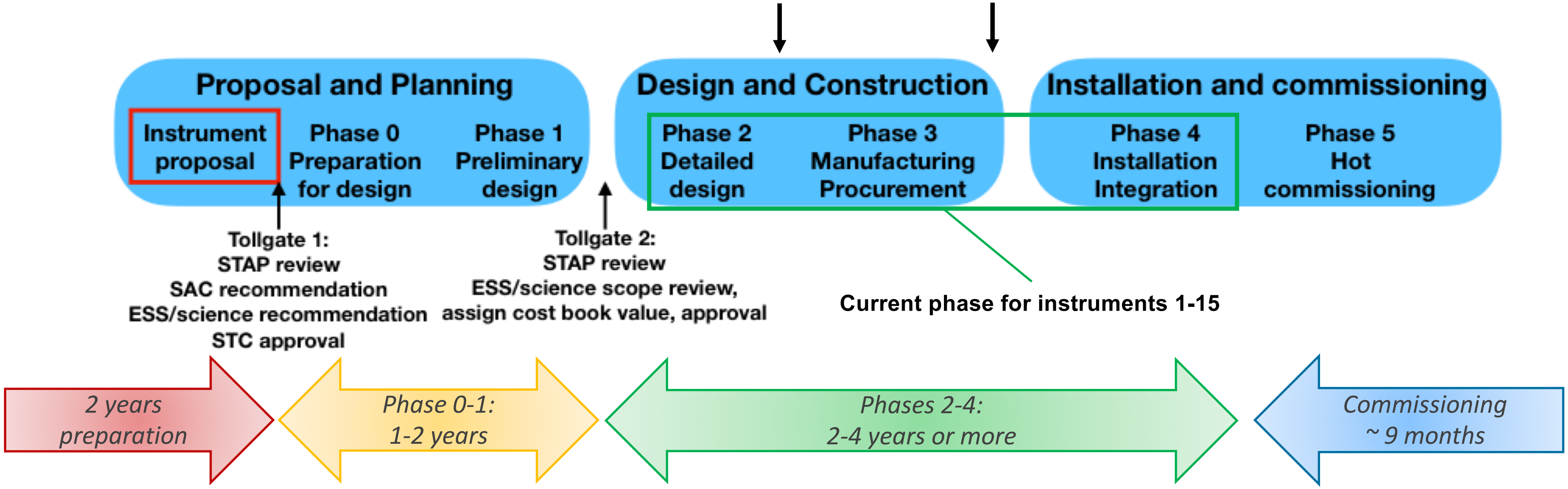
2021-05-12

New instruments at ESS

What is the process for proposing new instruments?

Process is a long one…



The more preparation done for the proposal the shorter phases 0-1

Instrument capability gap analysis

What is missing from the current instrument suite?

In 2018 ESS wrote a gap analysis report. This identified a number of instrument types that would be needed to complement the existing 15 instruments

High-Priority Capability Gaps

- Particle Physics
- High-Resolution Neutron Spin-Echo

Other Significant Capability Gaps

- High-Pressure Diffraction
- **Grazing-Incidence Small-Angle Neutron Scattering**
- Very Fast Spectroscopy
- Wide-Bandwidth Spectroscopy
- High Magnetic Fields

Lower-Priority Capability Gaps

- Bio-SANS
- Hydrogenous-Sample Diffraction
- Wide-Angle Neutron Spin-Echo

https://europeanspallationsource.se/instruments/capability-gap-analysis

EUROPEAN SPALLATION SOURCE

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THE ESS INSTRUMENT SUITE – A CAPABILITY GAP ANALYSIS

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Abstract

The 15 instruments currently under construction at ESS represent a subset of the full 22-instrument suite needed for the facility to reach its full scope, as defined in the ESS statues. In order to guide the selection of the remaining 7 instruments, we here provide an analysis of the missing capabilities.

SAGA: Surface Analyses using Grazing Angle neutron scattering

- A Swedish Instrument for Interface Science at ESS

Since 2015 the Swedish community has been building support for a Swedish led GISANS instrument at ESS

SAGA Swedish Instrument for Interface Science at ESS

[HOME] [ABOUT GISANS] [HISTORY] [ROADMAP] [SCIENCE CASE] [STEERING GROUP]

Welcome to the Open Meeting for a Swedish Surface Scattering Instrument Project for ESS

Sweden is currently making unprecedented investments in research infrastructures with the development and construction of the European Spallation Source (ESS) in Lund. To take full advantage of this great opportunity a lot of effort and funding is put into rebuilding, expanding and enhancing the Swedish scattering community and local neutron ecosystem. Swedish research groups from several universities are already involved in developments related to a broad spectrum science and technologies at future ESS. This is large performed with funding through the recent neutron project grants from the Swedish Research Council (VR). However, at current time none of the planned ESS neutron instruments are lead/planned/managed by a Swedish groups or collaborations.

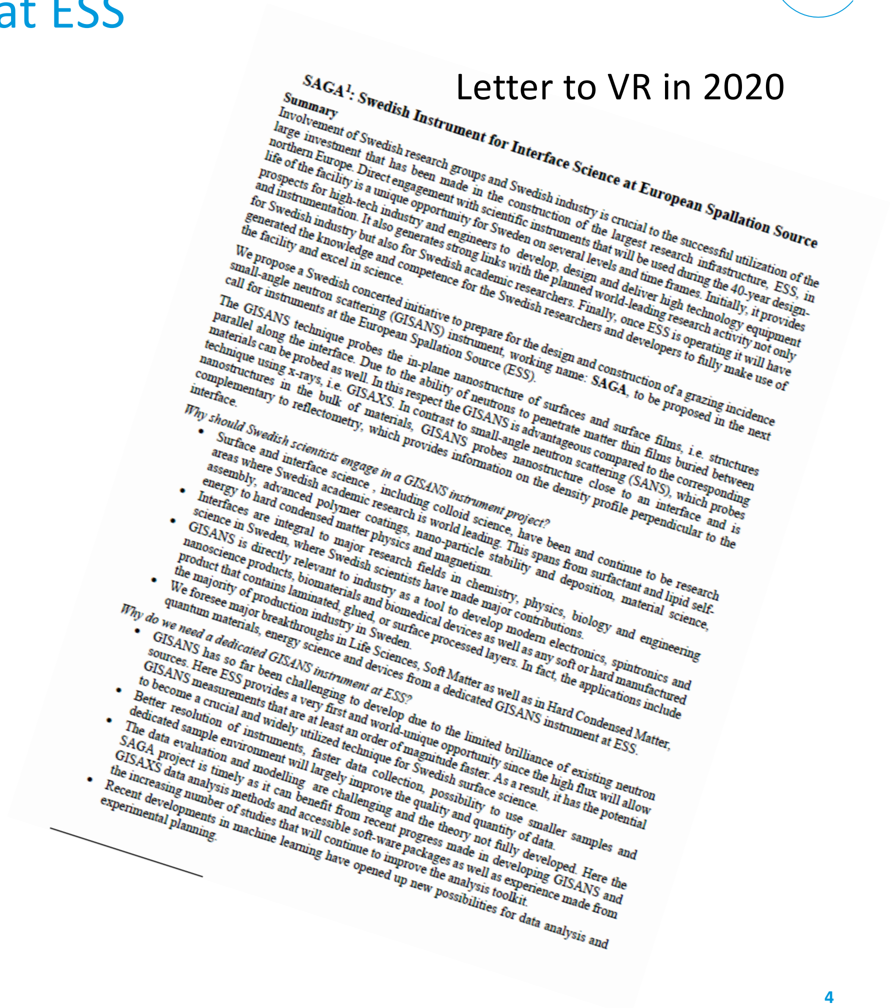
Recently it has been a general drive and wide interest in Sweden to move towards a Swedish instrument project for ESS. There are of course many options for which type of instrument that could best benefit the Swedish research community. Since a couple of years one specific suggestion has been put forward and that is focus on surface and interfaces with a surface scattering instrument, or in more specific a dedicated Grazing-Incidence Small-Angle Neutron Scattering (GISANS) instrument. The project goes under the working name SAGA (previously also known as GRAZE) and the idea was put forward mid 2015 and has since then been discussed at three workshops. SAGA has gained **support from a wide Swedish community** and currently 12 different Swedish institutions have joined forces to produce a National Science Case for SAGA.

Recent good news is that AstraZeneca has given its official support for the SAGA project. We very warmly welcome them to the team!

Further information about the process can be found in the menu links above.

Our Funding Partners:

Letter to VR in 2020



SAGA[1]: Swedish Instrument for Interface Science at European Spallation Source

Summary

Involvement of Swedish research groups and Swedish industry is crucial to the successful utilization of the large investment that has been made in the construction of the largest research infrastructure, ESS, in northern Europe. Direct engagement with scientific instruments that will be used during the 40-year design-life of the facility is a unique opportunity for Sweden on several levels and time frames. Initially, it provides prospects for high-tech industry and engineers to develop, design and deliver high technology equipment and instrumentation. It also generates strong links with the planned world-leading research activity not only for Swedish industry but also for Swedish academic researchers. Finally, once ESS is operating it will have generated the knowledge and competence for the Swedish researchers and developers to fully make use of the facility and excel in science.

We propose a Swedish concerted initiative to prepare for the design and construction of a grazing incidence small-angle neutron scattering (GISANS) instrument, working name: **SAGA**, to be proposed in the next call for instruments at the European Spallation Source (ESS).

The GISANS technique probes the in-plane nanostructure of surfaces and surface films, i.e. structures parallel along the interface. Due to the ability of neutrons to penetrate matter thin films buried between materials can be probed as well. In this respect the GISANS is advantageous compared to the corresponding technique using x-rays, i.e. GISAXS. In contrast to small-angle neutron scattering (SANS), which probes nanostructures in the bulk of materials, GISANS probes nanostructure close to an interface and is complementary to reflectometry, which provides information on the density profile perpendicular to the interface.

Why should Swedish scientists engage in a GISANS instrument project?

- Surface and interface science , including colloid science, have been and continue to be research areas where Swedish academic research is world leading. This spans from surfactant and lipid self-assembly, advanced polymer coatings, nano-particle stability and deposition, material science, energy to hard condensed matter physics and magnetism.
- Interfaces are integral to major research fields in chemistry, physics, biology and engineering science in Sweden, where Swedish scientists have made major contributions.
- GISANS is directly relevant to industry as a tool to develop modern electronics, spintronics and nanoscience products, biomaterials and biomedical devices as well as any soft or hard manufactured product that contains laminated, glued, or surface processed layers. In fact, the applications include the majority of production industry in Sweden.
- We foresee major breakthroughs in Life Sciences, Soft Matter as well as in Hard Condensed Matter, quantum materials, energy science and devices from a dedicated GISANS instrument at ESS.

Why do we need a dedicated GISANS instrument at ESS?

- GISANS has so far been challenging to develop due to the limited brilliance of existing neutron sources. Here ESS provides a very first and world-unique opportunity since the high flux will allow GISANS measurements that are at least an order of magnitude faster. As a result, it has the potential to become a crucial and widely utilized technique for Swedish surface science.
- Better resolution of instruments, faster data collection, possibility to use smaller samples and dedicated sample environment will largely improve the quality and quantity of data.
- The data evaluation and modelling are challenging and the theory not fully developed. Here the SAGA project is timely as it can benefit from recent progress made in developing GISANS and GISAXS data analysis methods and accessible soft-ware packages as well as experience made from the increasing number of studies that will continue to improve the analysis toolkit.
- Recent developments in machine learning have opened up new possibilities for data analysis and experimental planning.

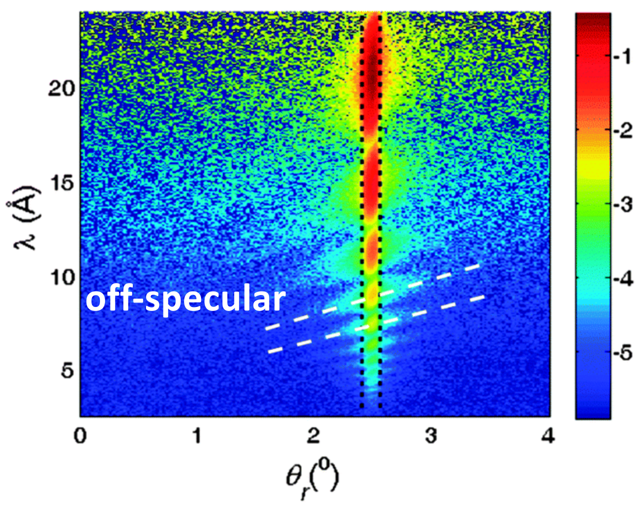
Neutron Reflectivity and GISANS

Specular reflectivitiy (Qz) probes the vertical structure with Å-resolution

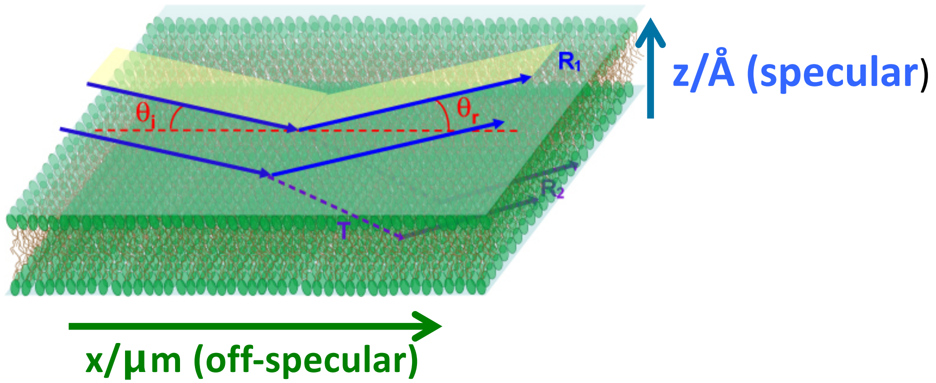
Off-specular reflectivity (Qx) probes µm-structures in the direction of the beam.

(limited by neutron coherence length)

specular $\theta_r = \theta_i$



Reflectivity (specular and off-specular) is measured with a divergent wide beam (cm) – this *averages lateral structure in y-direction*



D. James, A.M. Higgins, P. Rees, M. Geoghegan, M.R. Brown, S.-S. Chang, D. Mon, R. Cubitt, R. Dalgliesh, P. Gutfreund, Soft Matter, 11 (2015) 9393-9403.

Neutron Reflectivity and GISANS

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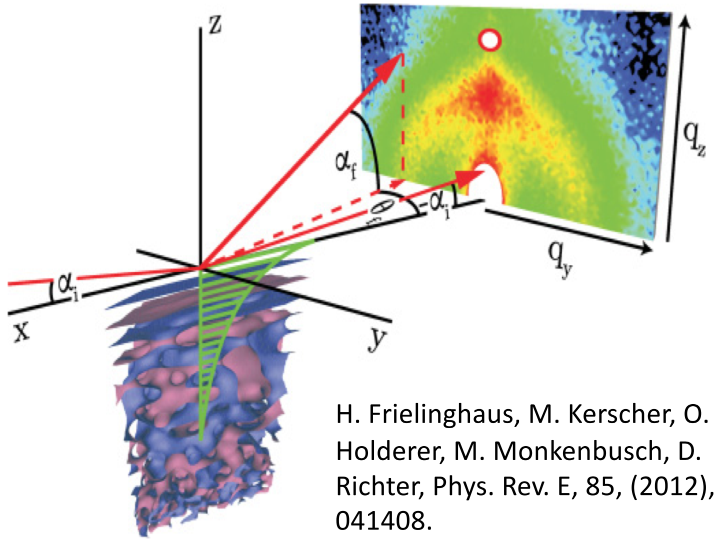
Off-specular reflectivity (Qx) probes µm-structures in the direction of the beam.

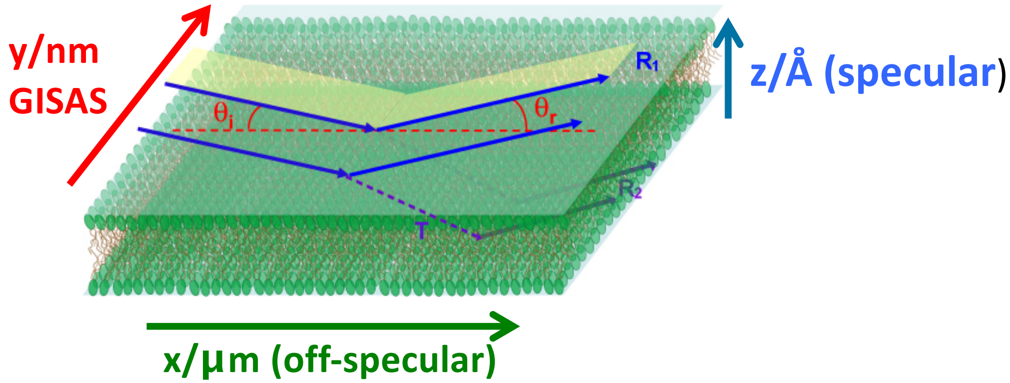
(limited by neutron coherence length)

Grazing Incidence SANS probes nm-structures in the y-direction.



H. Frielinghaus, M. Kerscher, O. Holderer, M. Monkenbusch, D. Richter, Phys. Rev. E, 85, (2012), 041408.

Reflectivity (specular and off-specular) is measured with a divergent wide beam (cm) – this *averages lateral structure in y-direction*



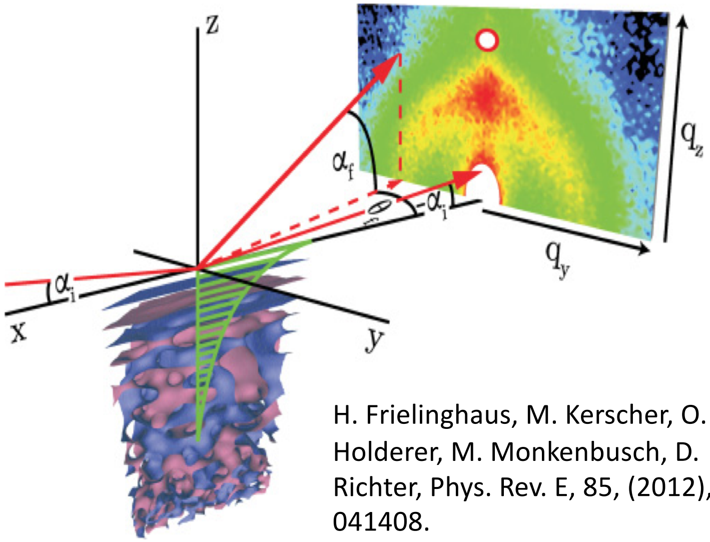
GISANS data is measured with **a narrow low-divergence beam** in the y-direction to *determine the 2D structure* in the sample plane => **Flux and background limited!**

Penetration depth:

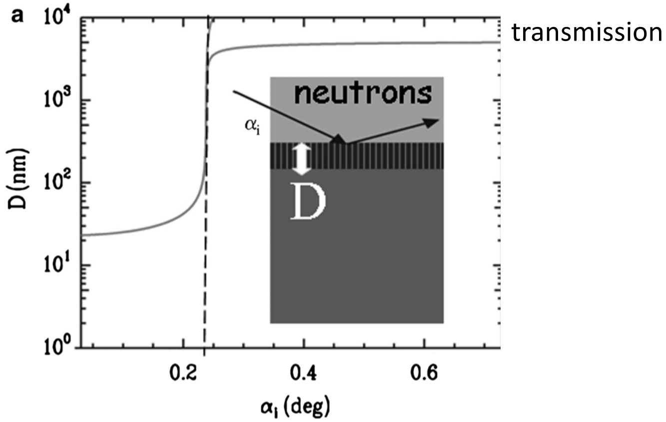
Below the angle of total reflection, an evanescent wave penetrates into the surface

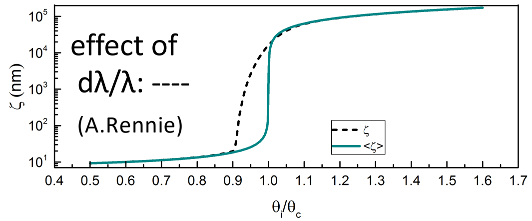
-> small angle scattering of reflected beam = surface sensitive

The penetration depth of neutrons is angle dependent:



H. Frielinghaus, M. Kerscher, O. Holderer, M. Monkenbusch, D. Richter, Phys. Rev. E, 85, (2012), 041408.

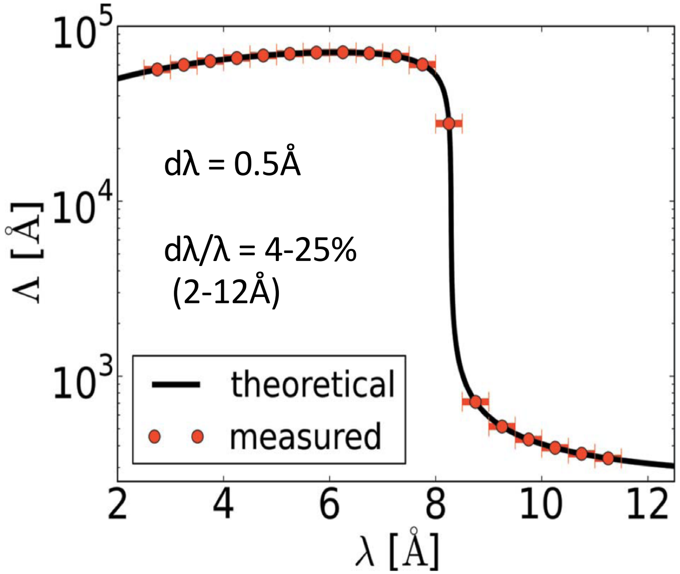




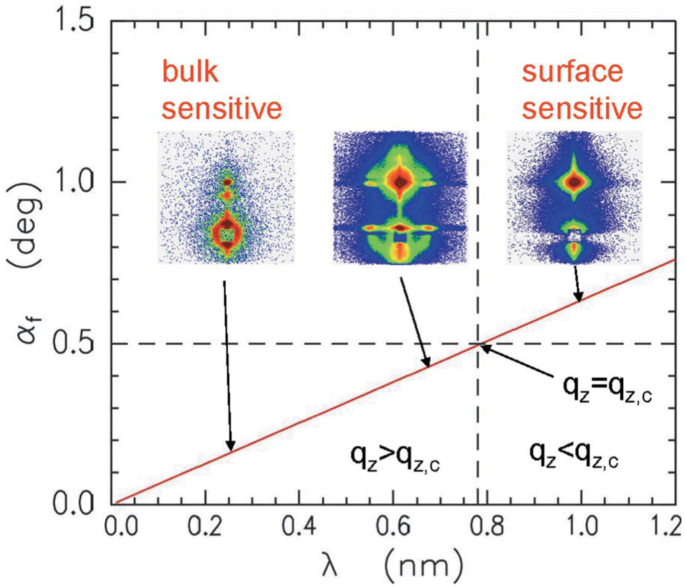
P. Mueller-Busch-Baum, Polymer Journal (2013) 45, 34–42

Time-of-flight GISANS

The penetration depth (~10-1000nm) of neutrons is also wavelength dependent:
- resolution dλ/λ important



True surface sensitivity only above critical wavelength/angle



P. Mueller-Buschbaum et al., J. Appl. Cryst. (2014). 47, 1228–1237

Requirements for a GISANS instrument

What capabilities are needed?

A GISANS instrument

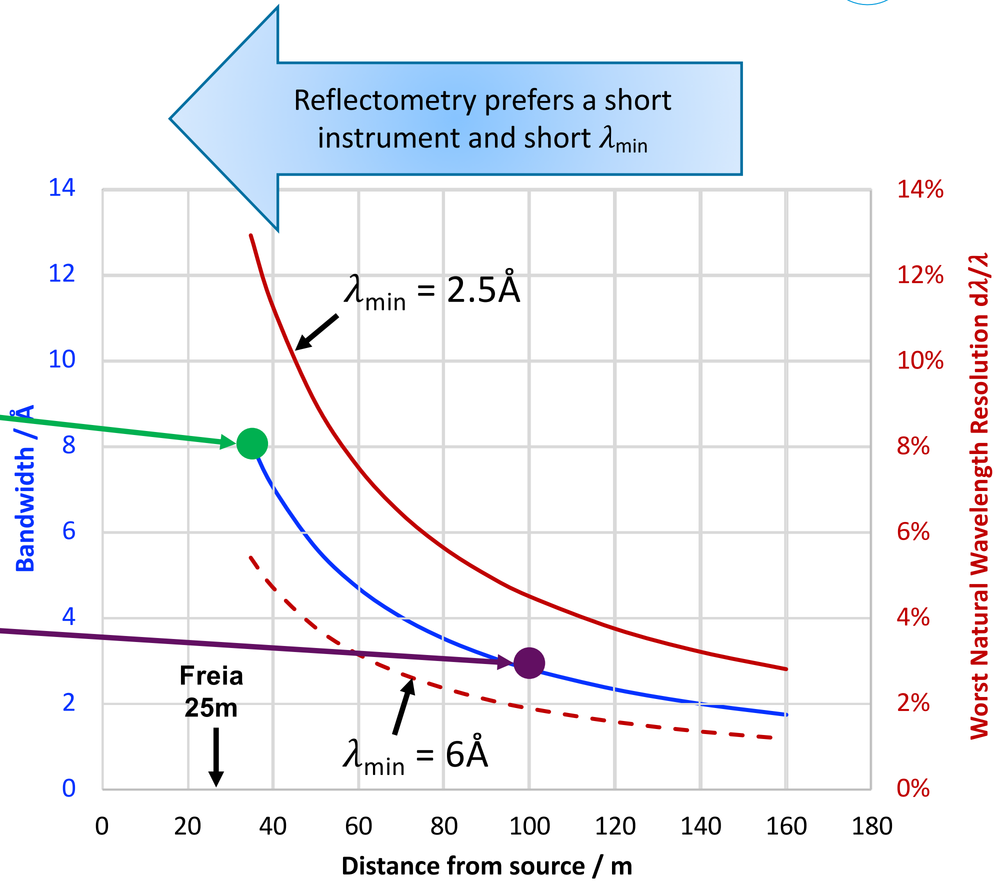
- will require **high flux**
- should be able to **measure reflectivity** up to about Qz = 0.35 $Å^{-1}$
- should be capable of accessing samples with **horizontal surfaces** or in **magnetic fields**
- have variable resolution (from around **7% to 1-2%**)
- have a **low background**
- have a flexible and spacious sample area for complex sample environments
- should allow for wide-angle detectors for GIWANS

Optimal wavelength & instrument length

For reflectometry

Reflectometry requires a **short minimum wavelength** and / or a **wide bandwidth**

- TOF Reflectivity curve is usually measured using 3-4 incident angles.
- For a bandwidth of 8Å
  - 3 angles to cover 0.007Å^{-1} – 0.35Å^{-1} with λ_{min} = 2.5Å
  - 5 angles to cover 0.007Å^{-1} – 0.35Å^{-1} with λ_{min} = 6Å
- For a bandwidth of 3Å
  - 6 angles to cover 0.006Å^{-1} – 0.35Å^{-1} with λ_{min} = 2.5Å
  - >9 angles to cover 0.006Å^{-1} – 0.35Å^{-1} with λ_{min} = 6Å

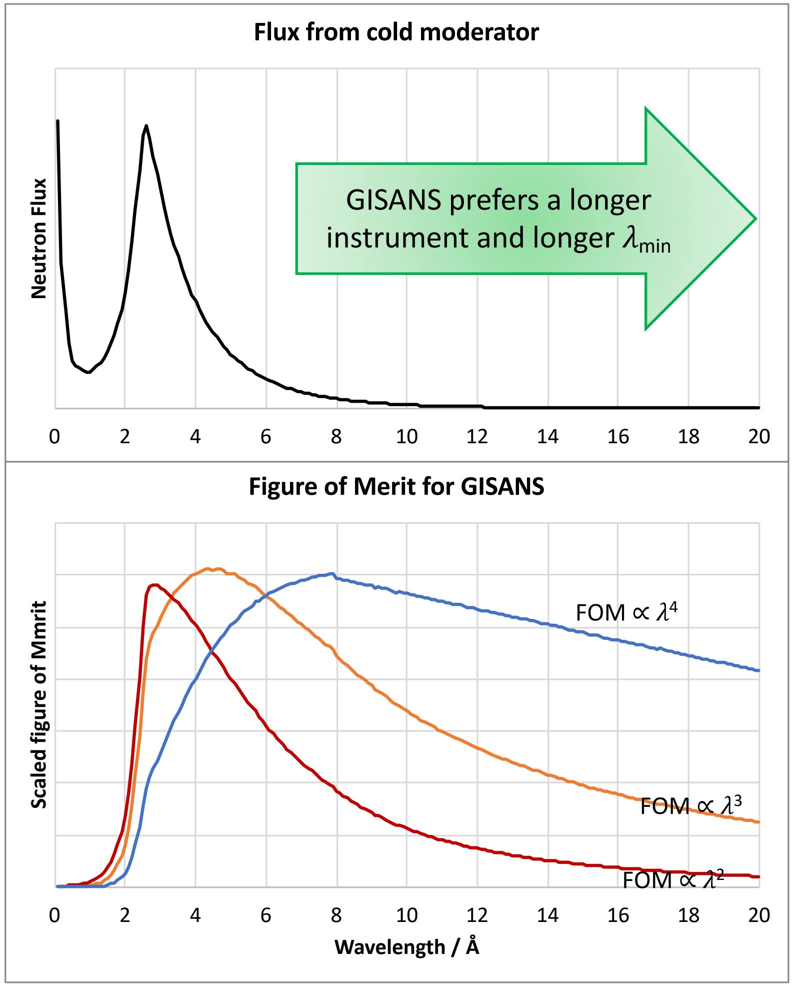


Optimal wavelength & instrument length

For GISANS

GISANS requires a longer minimum wavelength

- This is essentially because GISANS needs high Q resolution both in-plane and out-of-plane.
  - resolution improved for longer wavelengths
  - some other advantages e.g. for accessing buried interfaces.
- Define a Figure Of Merit: $FOM \propto I \times \lambda^4$
  - The peak flux from ESS cold moderator is ~2.6Å
  - Multiply this by FOM => ideal wavelength ~6-8Å
- GISANS also prefers a wide bandwidth but less important than for reflectivity
- Longer instrument gives better natural resolution
- Wavelength frame multiplication? – big loss of flux



Summary of requirements

A GISANS instrument will have to balance the needs for GISANS & NR

GISANS

- Min wavelength = 6-8Å
- Best Qz & Qxy resolution = 2-3%
- Good horizontal & vertical collimation
- High flux
- Low-background
- 4Å Bandwidth acceptable
- Downward trajectory for liquid surfaces – only 1 angle required

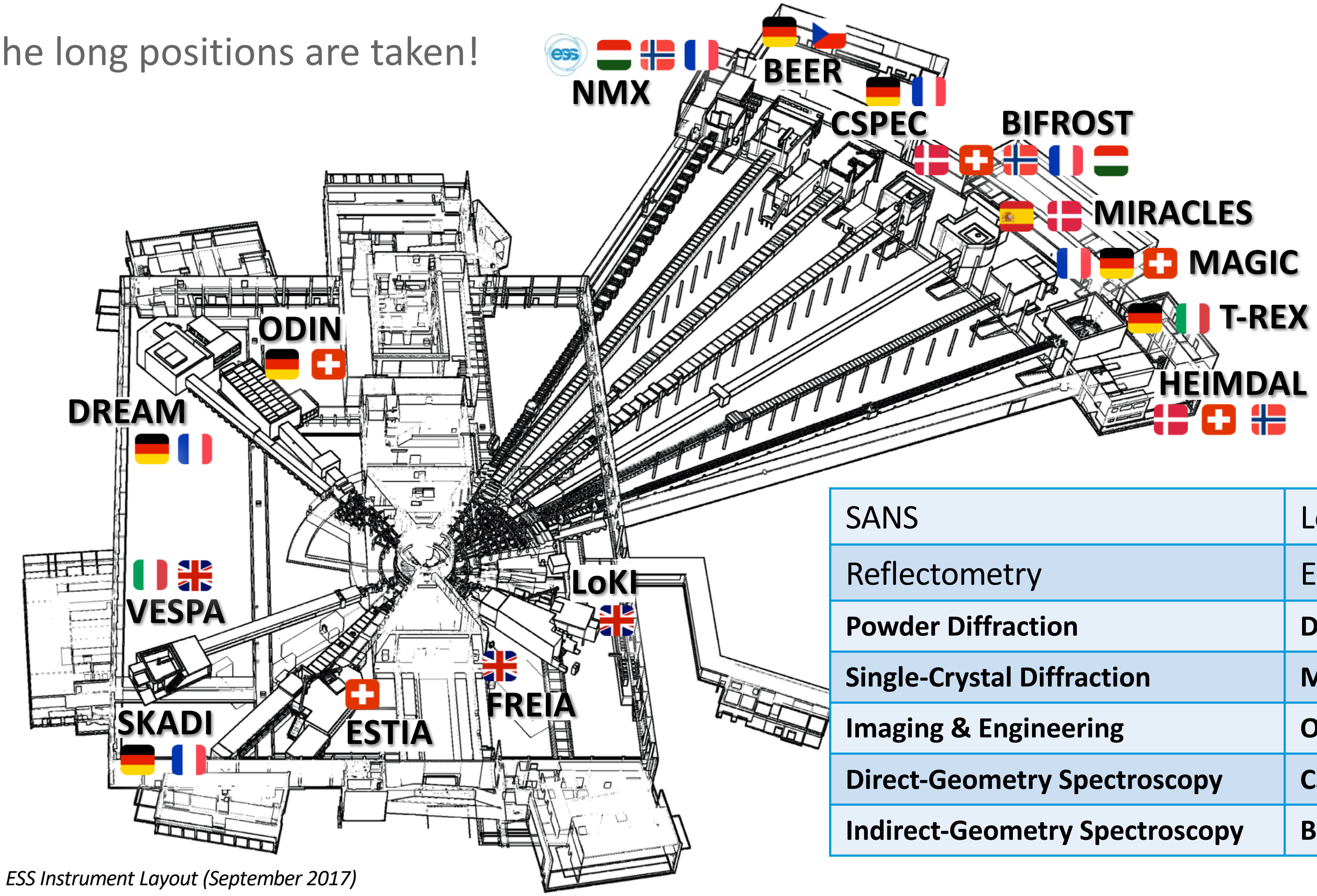
Reflectivity

- Min wavelength = 2-3Å
- Best Qz resolution = 2-3%
- Good collimation in vertical plane only
- High flux
- Low-background
- Bandwidth as long as possible
- Downward trajectory for liquid surfaces – at least 3 angles required

ESS Instrument Suite:

Where could a GISANS instrument go?

All the long positions are taken!



ESS Instrument Layout (September 2017)

SANS	LoKI, *SKADI*
Reflectometry	ESTIA, FREIA
Powder Diffraction	**DREAM**, HEIMDAL
Single-Crystal Diffraction	**MAGIC**, *NMX*
Imaging & Engineering	**ODIN**, **BEER**
Direct-Geometry Spectroscopy	**CSPEC**, *T-REX*
Indirect-Geometry Spectroscopy	**BIFROST**, MIRACLES, VESPA

Limitations at ESS

What distance is possible?

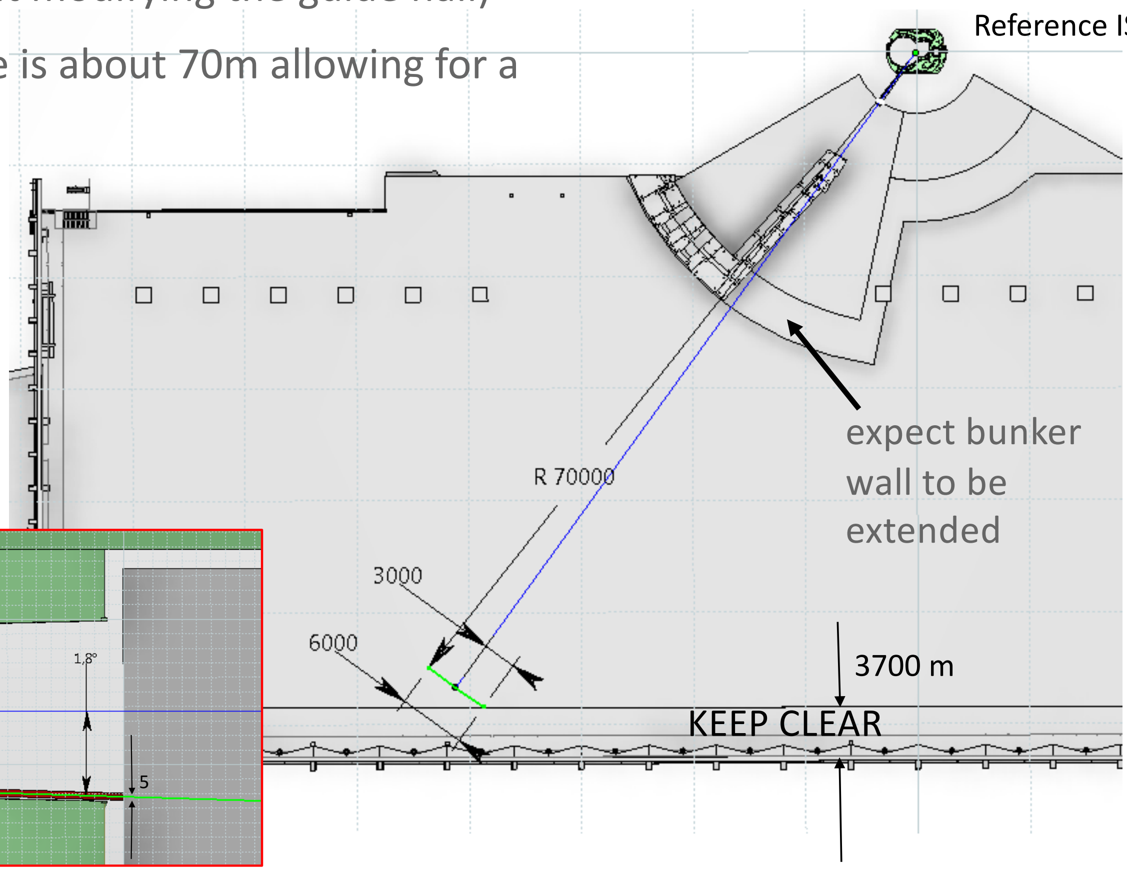
The longest instrument possible (without modifying the guide hall)

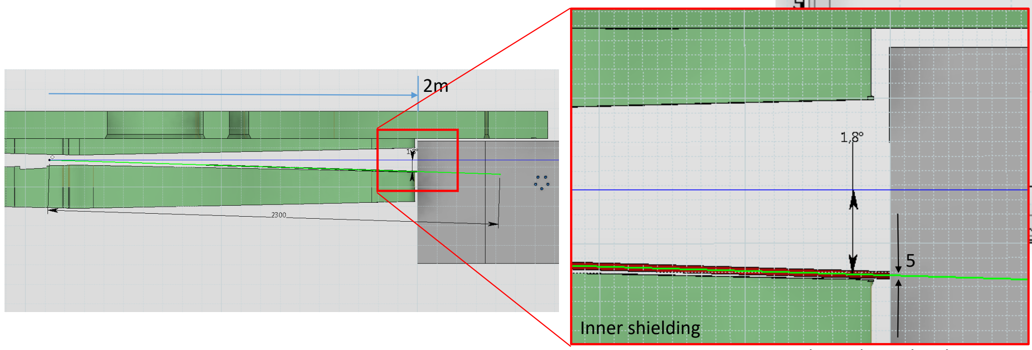
- Beam port S5 – max detector distance is about 70m allowing for a cave

For 6Å minimum wavelength at 70m

- bandwidth = 4Å
- natural λ resolution is 2-3%

Monolith has limitation on minimum exit angle: approx. 1.8˚





Considering beam height 5mm

Acknowledgements

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