



# SAGA

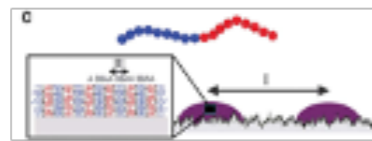
## An initiative for a GISANS instrument at the ESS

A concerted Swedish initiative based on the close collaboration and joint efforts of all the main Swedish research institutions with neutron activities and funded by the Swedish research council.

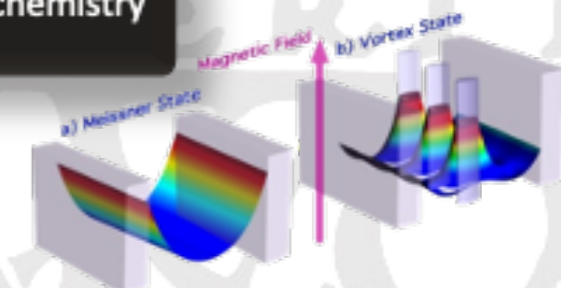
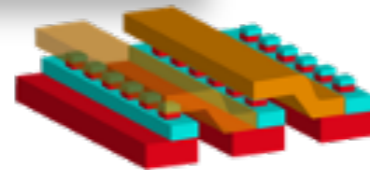
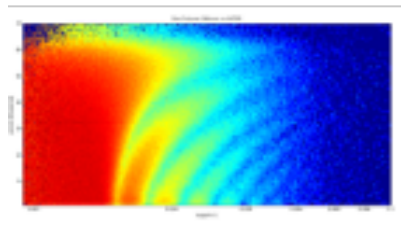
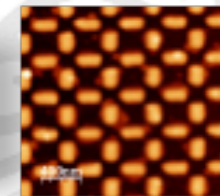
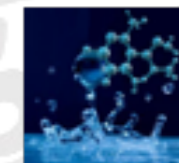
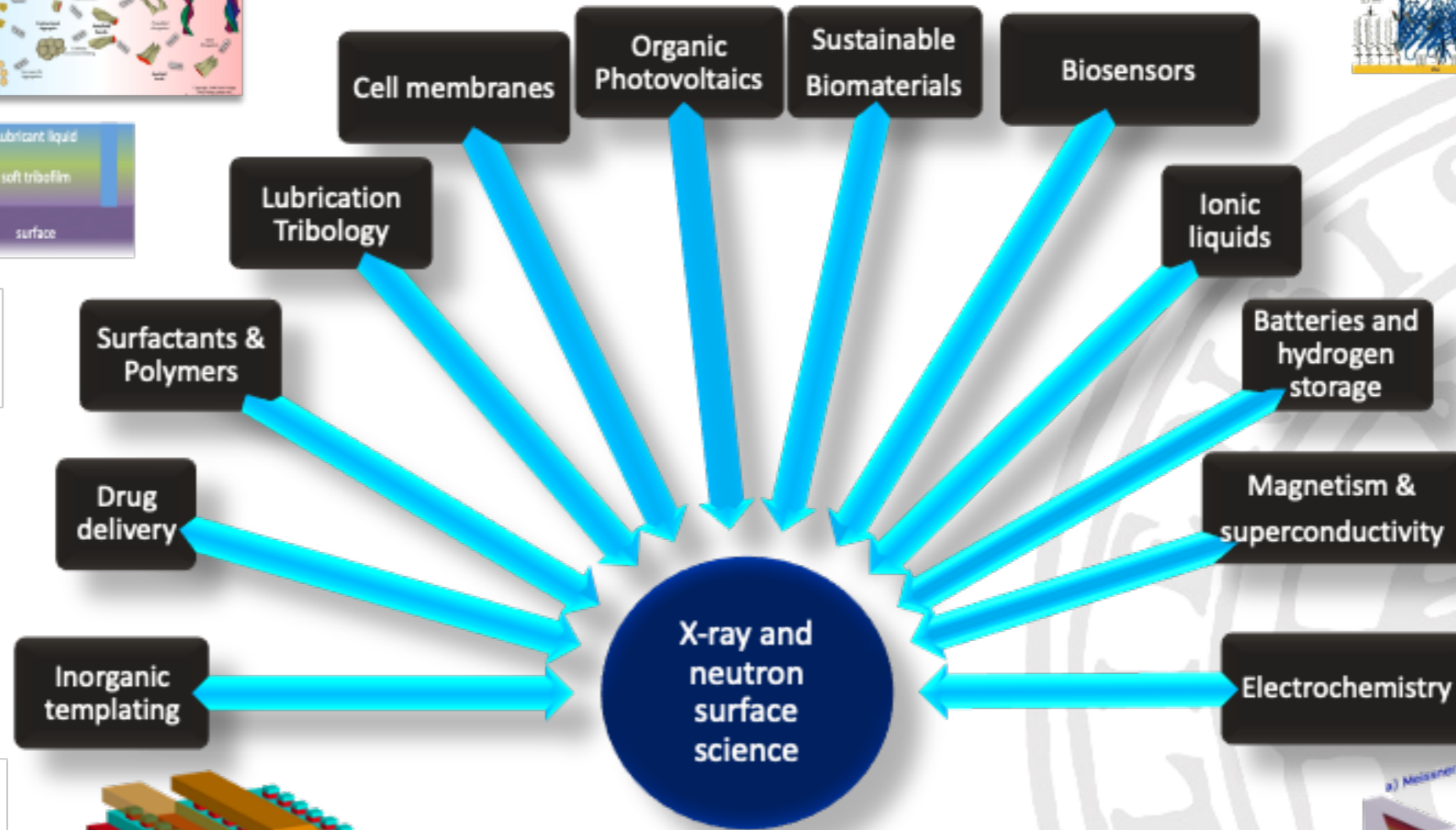
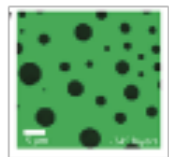
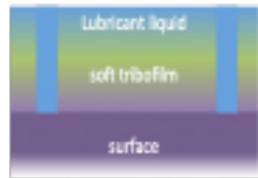
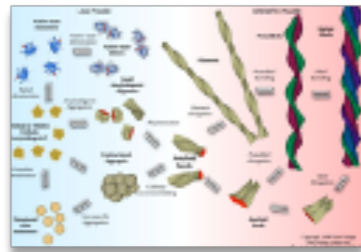
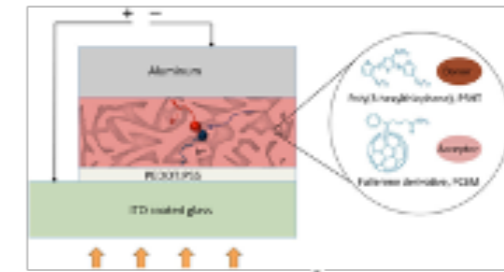
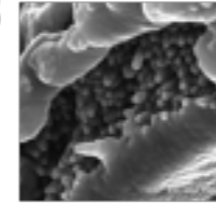
Goal: Competitive instrument proposal to ESS



# Surface science with neutrons



A Wide Range of Science involves  
- gas, liquid, solid interfaces





# Bibliometric study (Sweden)

**Table 2.** Number of publications divided with respect to neutron scattering technique over the time periods 2006–2010, 2011–2015 and 2016–2020 [4].

Technique/time period	2006–2010	2011–2015	2016–2020
Diffraction <sup>1</sup>	101	79	109
Reflectometry	30	54	92
SANS	35	68	99
Inelastic scattering	20	51	71
Imaging	1	8	35
Instrumentation	7	51	58
Stress	11	17	16
Other <sup>2</sup>	56	73	52
Total	261	401	532

Double counts may occur if more than one technique is used in one article.

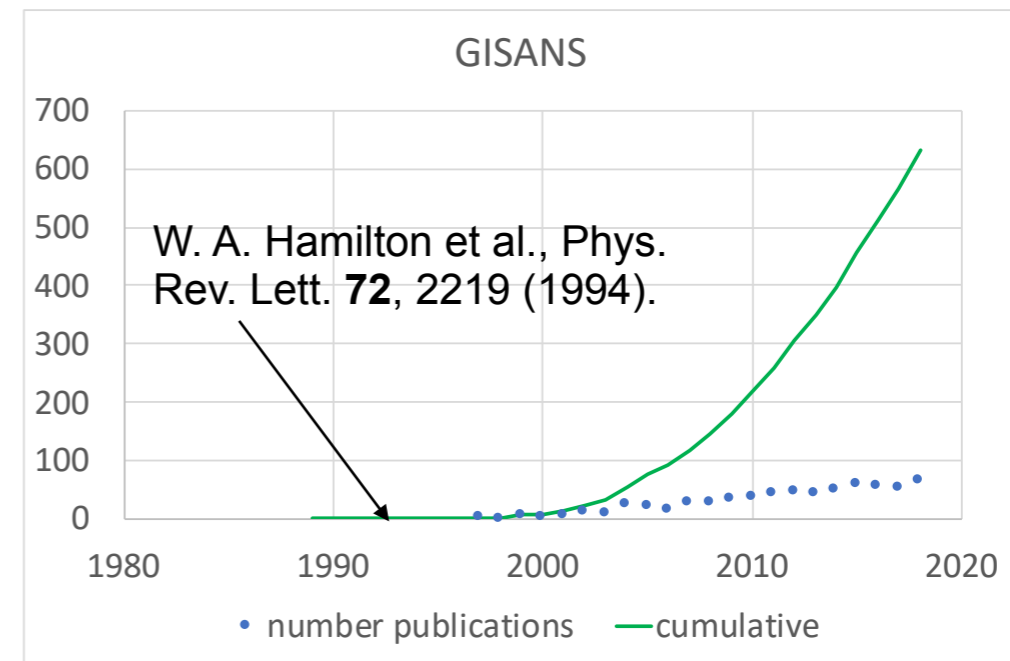
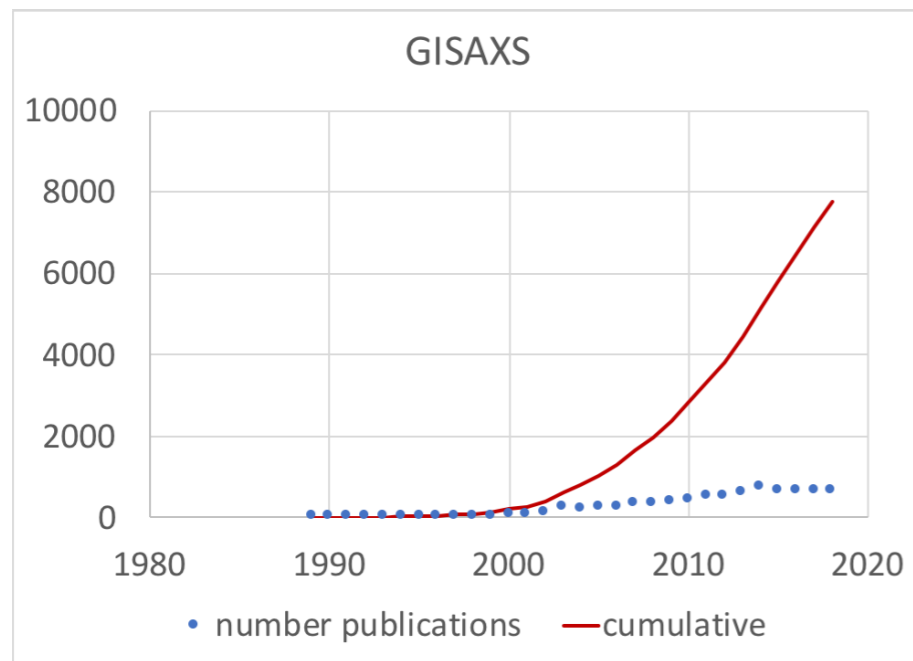
<sup>1</sup>Search terms: single crystal diffraction, powder diffraction, diffraction studies.

<sup>2</sup>Search terms: books, reviews, editor, crystallography, and theory.

Hanna Barriga, Marité Cárdenas, Stephen Hall, Maja Hellsing, Maths Karlsson, Adriano Pavan, Ru Peng, Nanny Strandqvist & Max Wolff (2021) A Bibliometric Study on Swedish Neutron Users for the Period 2006–2020, *Neutron News*, 32:4, 28-33, DOI: 10.1080/10448632.2021.1999147



# Background - GISANS

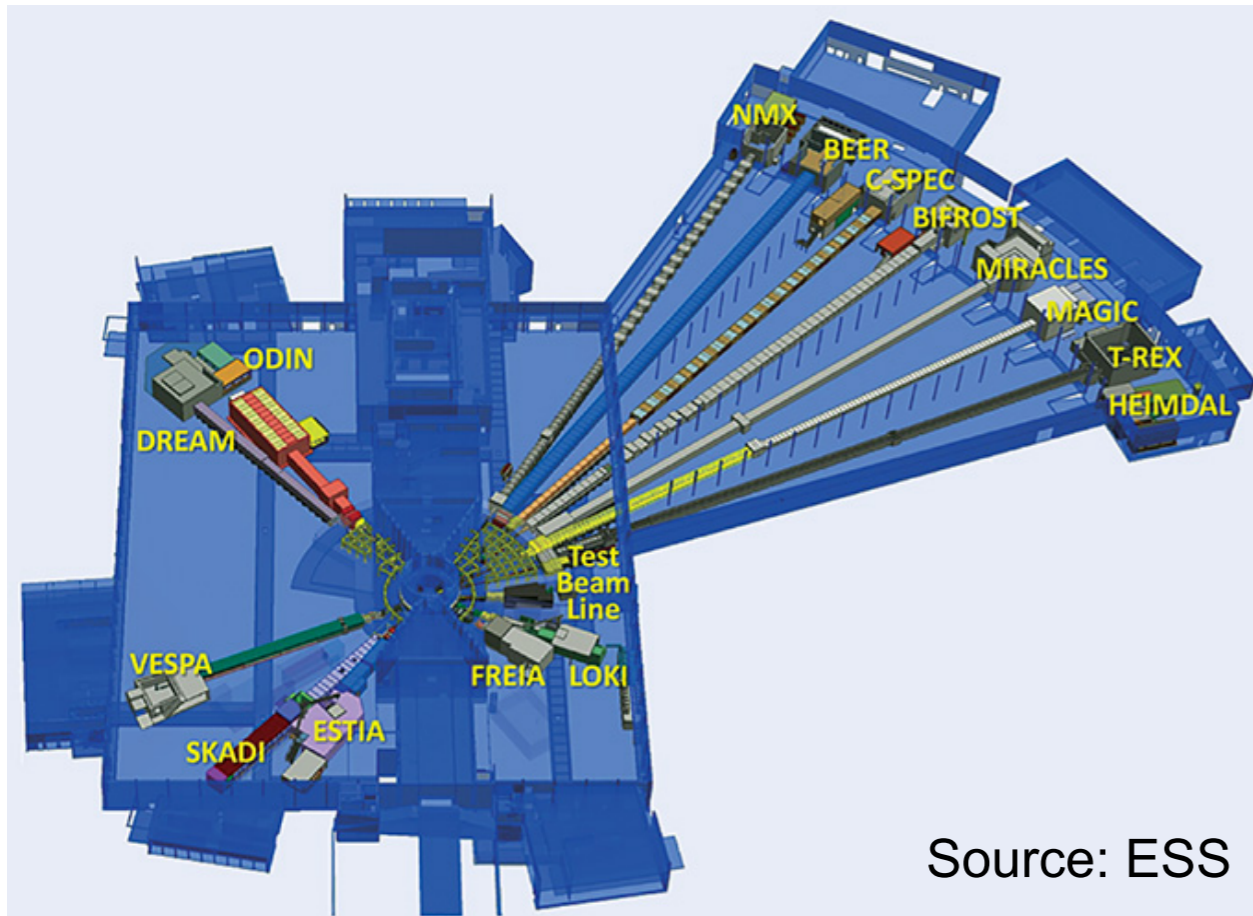


Instrument	Facility	Type	Detector dist.	Comment
D22	ILL	SANS	up to 18m	Monochromatic SANS
SANS2D	ISIS	SANS		ToF SANS
KWS2	FRM2	SANS	up to 20m	Pinhole SANS
Figaro	ILL	Reflectometer	3m	Horizontal
REFSANS	FRM2	Reflectometer	up to 12m	Horizontal*, Focusing
PA20	LLB	SANS		Facility closing 2019
MARIA	FRM2	Reflectometer	4m	Polarised
SuperADAM	ILL	Reflectometer	8m	Polarized, Swedish CRG

The only dedicated GISANS beamline REFSANS faces design challenges



# Instrumentation at ESS



Source: ESS

## 15 instruments under construction:

Diffraction: DREAM, HEIMDAL, MAGIG, NMX

Engineering and diffraction: BEER, ODIN

Large Scale Structures: ESTIA, FREIA, LoKI, SKADI

Spectroscopy: BIFROST, CSPEC, MIRACLES, T-REX, VESPA

## Plan and space for instruments 16-22

**Possible future expansion to 35 instruments**

## ESS capability gaps:

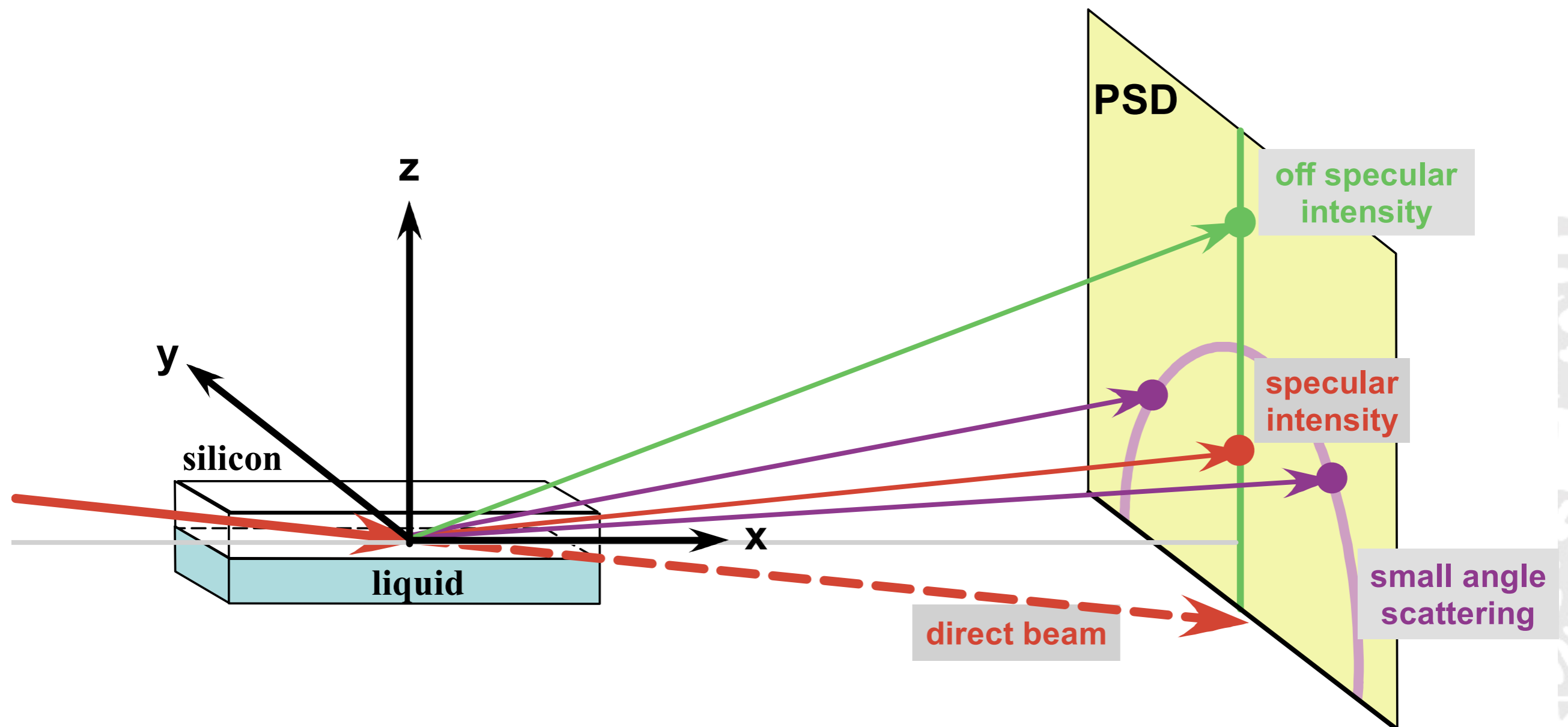
Priority 1 (good existing proposals / no funding): Fundamental physics, High resolution NSE

Priority 2: High-pressure diffraction, Very fast spectroscopy, Wide bandwidth spectroscopy, High magnetic fields, **Grazing incidence SANS**

Priority 3: Bio-SANS, Hydrogenous sample diffraction, Wide angle spin echo



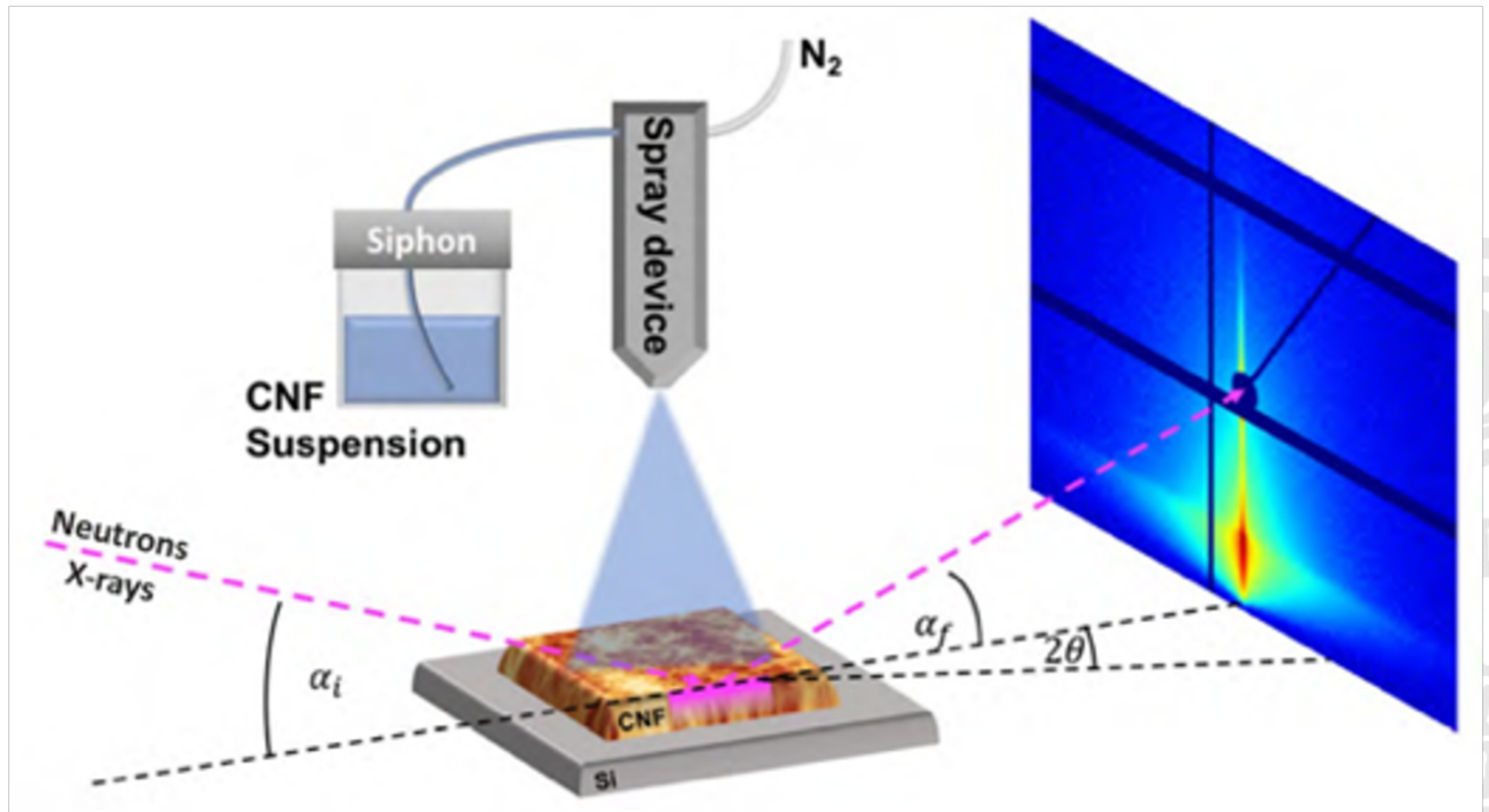
# Scattering geometry



Grazing incidence scattering,  
in: French-Swedish winterschool on neutron scattering: Applications to soft matter Eds.: M. Wolff, F. Cousin  
EPJ Web of Conferences **188**, 04002 (2018).



# Drying of cellulose coatings

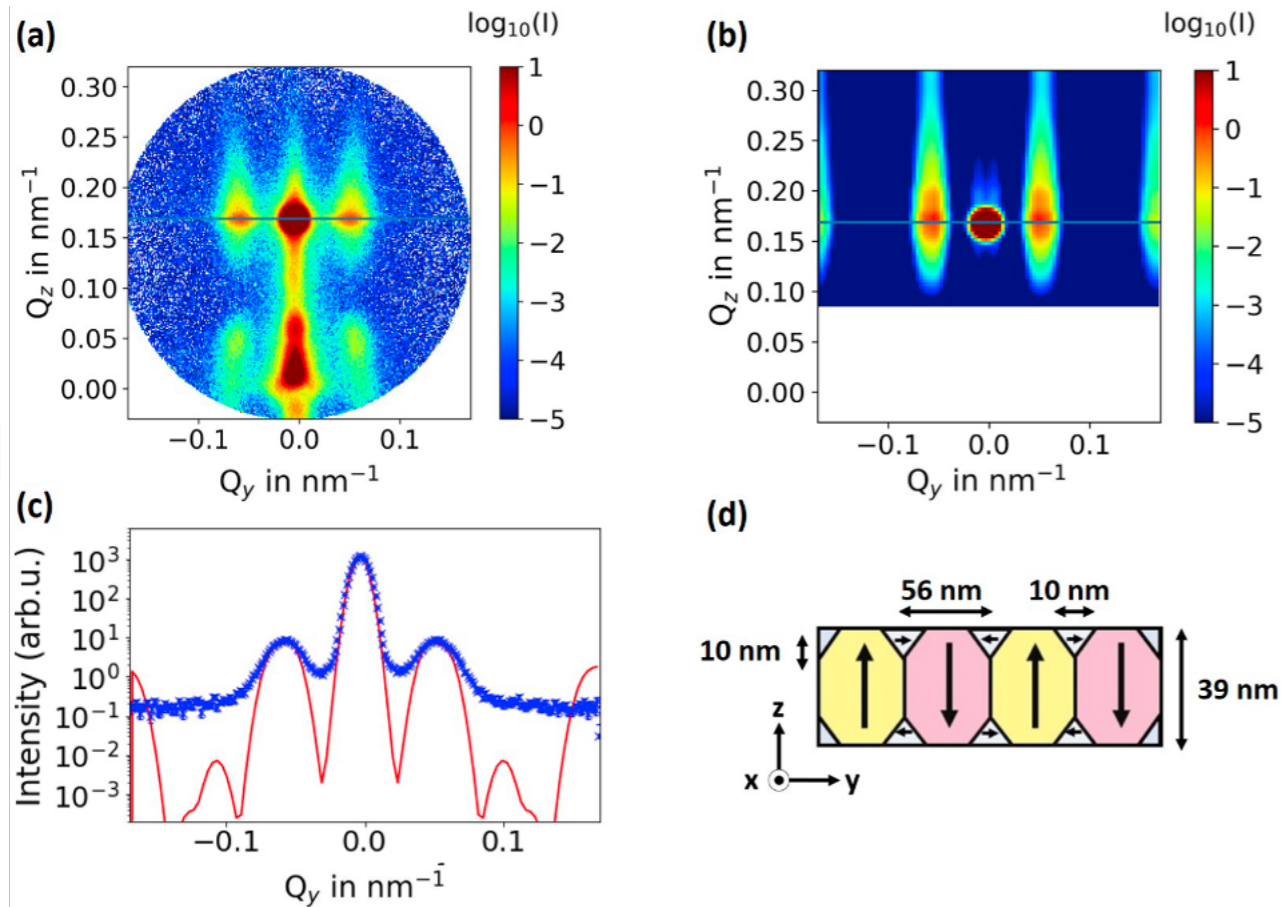


C. J. Brett et al.,

Water-Induced Structural Rearrangements on the Nanoscale in Ultrathin Nanocellulose Films  
Macromolecules 52, 12, 4721-4728 (2019)



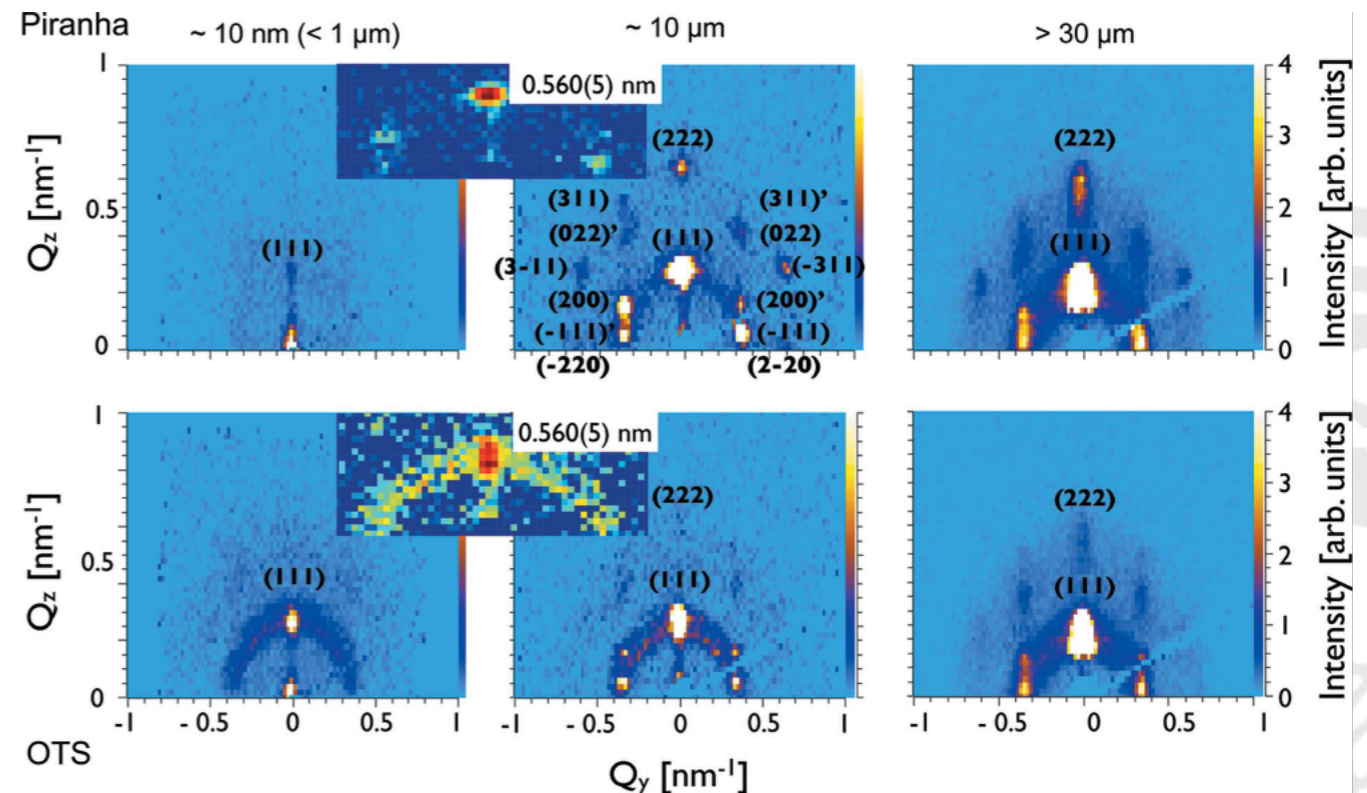
## Hard matter



Magnetic scattering from a FePd thin films with strong perpendicular magnetic anisotropy (panel a).

Simulations (panel b) using the DWBA reveal the magnetic domain structure.

## Soft matter



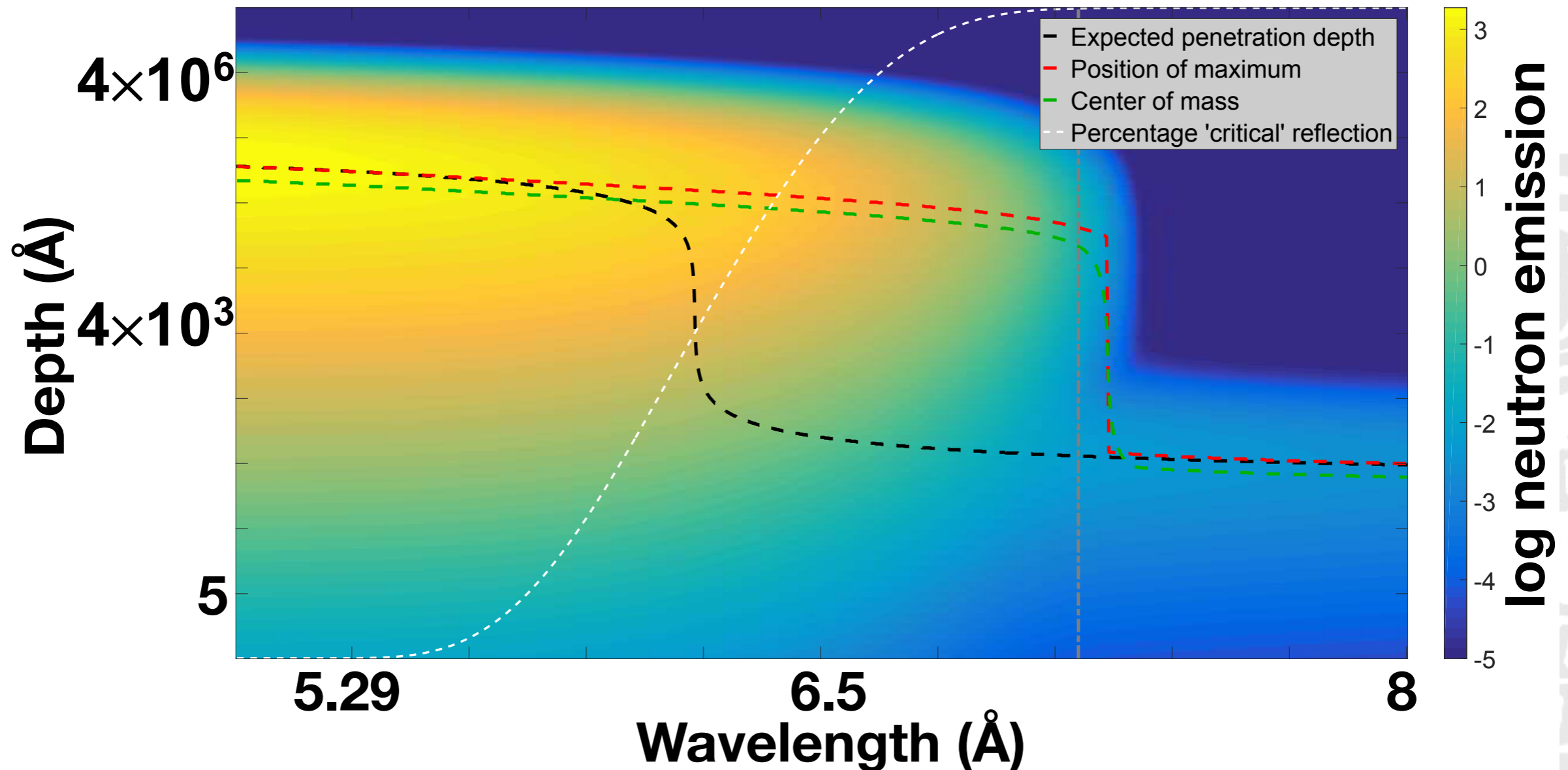
Depth resolved structure of polymer micelles in contact with differently treated silicon surfaces.

The panels to the left highlight the need of high resolution to distinguish surface from bulk scattering.



# Effect of resolution

Scattering from beyond a semi-infinite interface



For GISANS high resolution is required (ideally 1 %)

For reflectometry and SANS the resolution may be relaxed (typically 10 %)



## A GISANS instrument:

- will require **high flux**
- should be able to **measure reflectivity** up to about  $Q_z = 0.35 \text{ \AA}^{-1}$
- 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

## Current/initial idea:

Optimise for high resolution/brilliance (long instrument) GISANS on the expense of band width

Provide second beam of lower resolution larger bandwidth for reflectometry.



## Within Sweden:

**Strong collaborative network** including almost all Swedish Universities and institutions, e.g. KTH, LU, UU, RiSE, LiU, Chalmers, MaU, SU, GU, MiU, LTU and UMU

**Industrial interest** from e.g. AstraZeneca, Sandvik, ABB, AlfaLaval, Tetra Pak and many small companies like Epiluvac

**Educational and community efforts** by SwedNess and SNSS

## Connection to the international GISANS community:

**Experts from neutron laboratories** (PSI, MLZ, JCNS, STFC-ISIS, LLB, ESS) participate in meetings to define the instrument scope and design criteria.

**Competence building** at ISIS, NCNR (NIST) and ESS.

**Collaborative projects**, e.g., ILL (Super ADAM) and MLZ (Port-GISANS and surface dynamics)



UPPSALA  
UNIVERSITET

# Project organisation

**Coordination** with team members, the science and industry community and the funding bodies: T. Nylander (LU)

**Conceptual and technical design** + evaluate alternative and innovative instrument concepts: M. Wolff (UU)

**Interface to the ESS** and ensure integration into the ESS instruments suite and development: T. Arnold (ESS)

## **Working groups:**

**Technical developments:** J. Birch (LiU)

**International experts** group: S. Rogers (ISIS), S. Roth (Desy)

**Swedish user** community: M. Månsson (KTH), M. Cárdenas (MaU)

**International user** community: Adrian Rennie (UU)

PostDoc1 (Design), Sebastian Köhler recruited and stationed at LINXS

PostDoc2 (Technical developments, recruitment ongoing)

Engineer (Drawings, 30 % over three years)



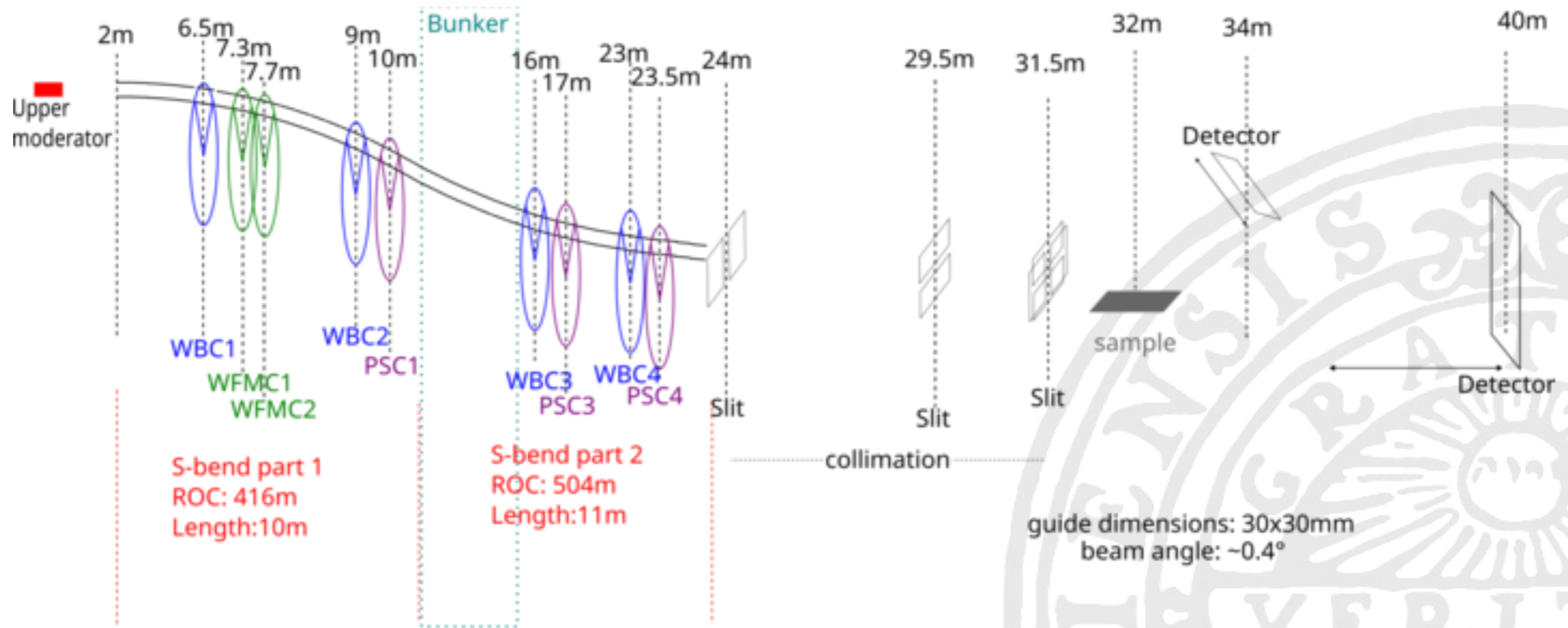
# Timeline

	Q4-21	Q1-22	Q2-22	Q3-22	Q4-22	Q1-23	Q2-23	Q3-23	Q4-23	Q1-24	Q2-24	Q3-24	Q4-24
Recruitment	█												
Preparatory work	█	█											
Conceptual design (WP1)		█ D1.1	█ D1.2	█ D1.3									
Task 1.1 Update Science Case		█											
Task 1.2 Define Technical Spec.		█	█										
Task 1.3 Define Concept				█									
Task 1.4 Feasibility studies		█	█	█									
Technical design (WP2)				█ D2.1	█ D2.1	█ D2.1	█ D2.1	█ D2.1	█ D2.1	█ D2.1	█ D2.1		
Task 2.1 Detailed simulations				█	█				█	█	█		
Task 2.2 Prototyping					█	█	█						
Task 2.3 Performance tests							█	█	█				
Task 2.4 Technical details									█	█	█		
Proposal writing (WP3)										█	█ D3.1	█ D3.2	█ D3.3
Task 3.1 Science case & overview									█	█			█
Task 3.2 Budget										█	█	█	
Task 3.3 Project planning												█	█
Coordination & Engagement (WP4)	█ D4.1	█ D4.2	█ D4.2	█ D4.2	█ D4.2	█ D4.2	█ D4.2	█ D4.3	█ D4.3	█ D4.3	█ D4.3	█ D4.4	█ D4.4
Kick-off meeting	█												
Regular SAGA partner meetings		█	█		█	█	█		█	█	█		█
SAGA GISANS Workshops				█				█				█	





# Short instrument (40 m)

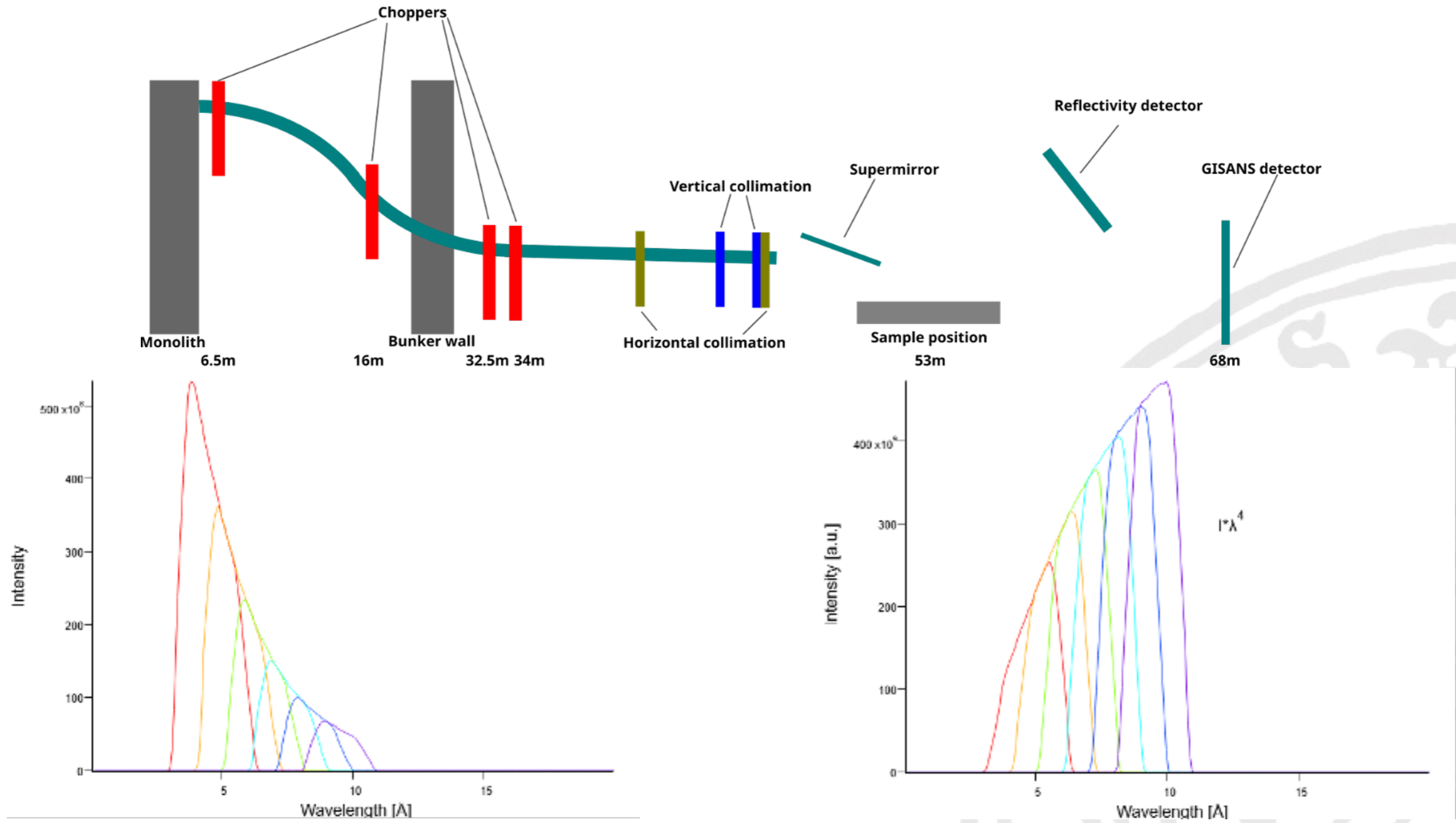


No WFM: Resolution 9-3%, Bandwidth: 3 -10 Å, Flux:  $2 \cdot 10^9$  n/s/cm<sup>2</sup>

WFM: Resolution 1.3 %, Bandwidth: 4-10 Å, Flux:  $3.2 \cdot 10^8$  n/s/cm<sup>2</sup>



# Long instrument (70 m)

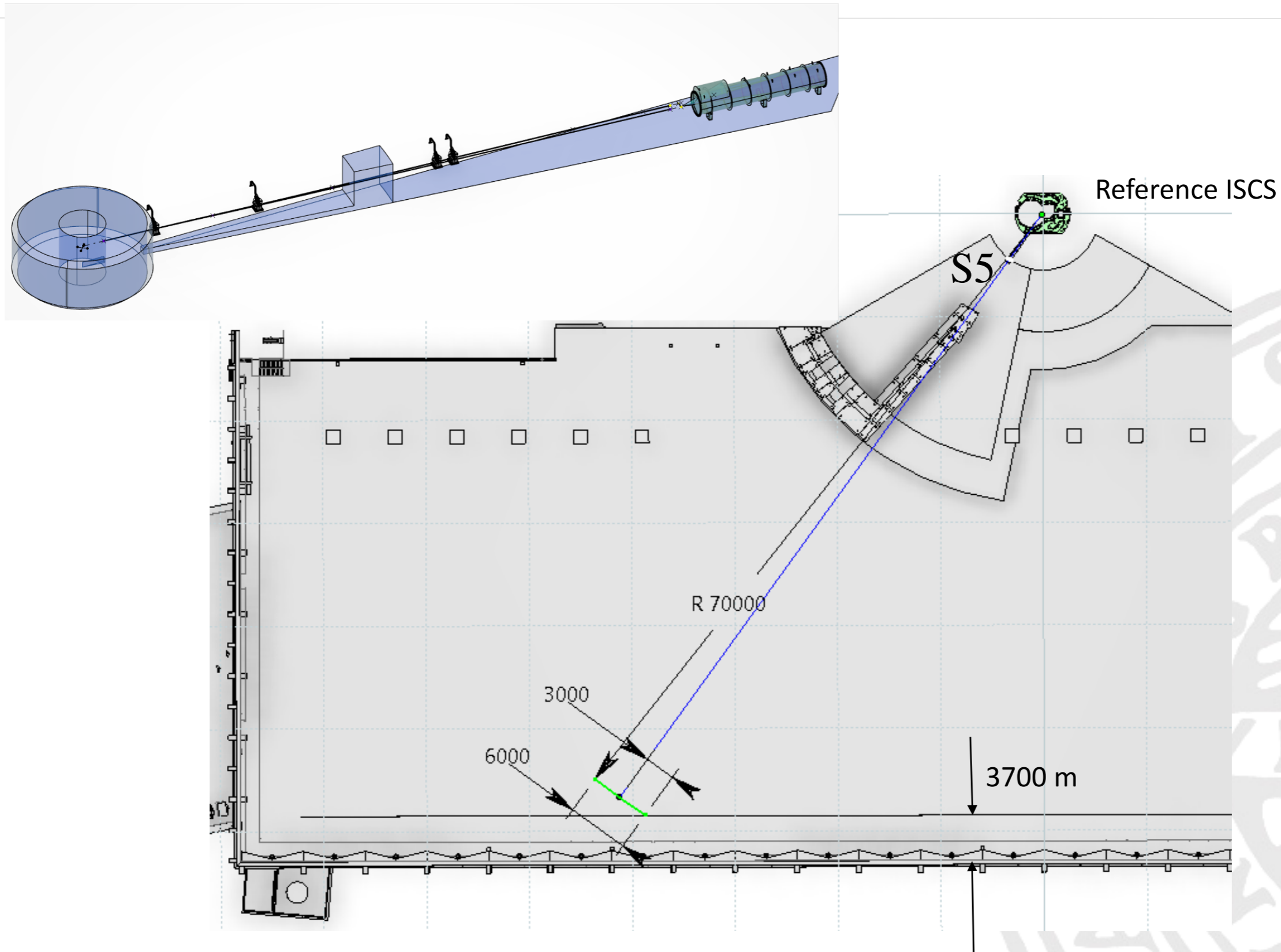


Resolution 4-2%, Bandwidth: 4 - 8  $\text{\AA}$ , Flux:  $2 \times 10^9$  n/s/cm<sup>2</sup>

Separate reflectometry guide?

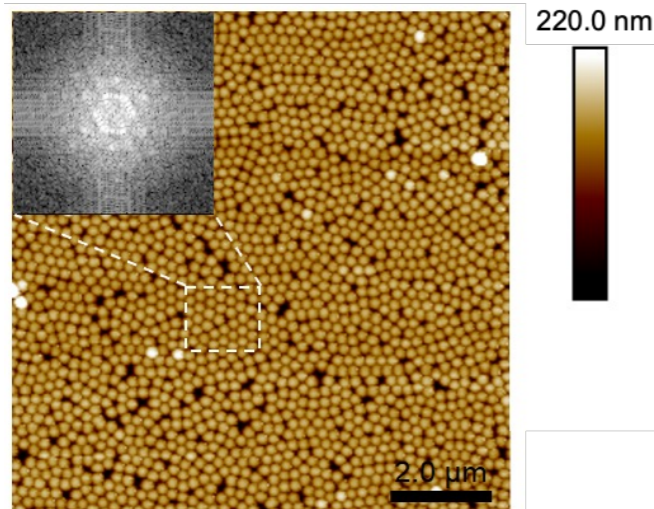


# Possible position

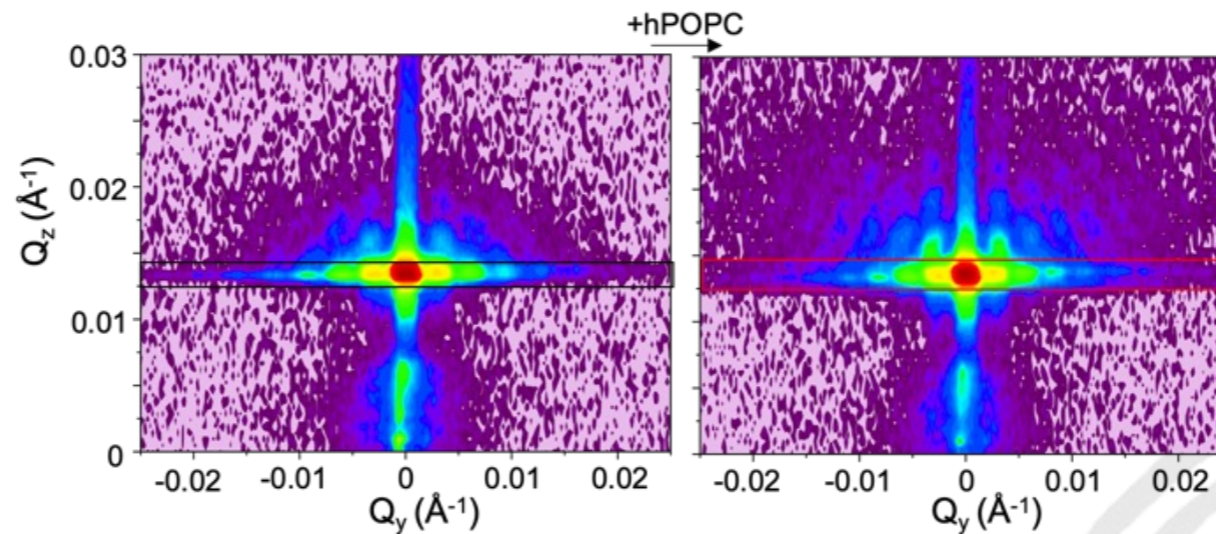




## Benchmarking:



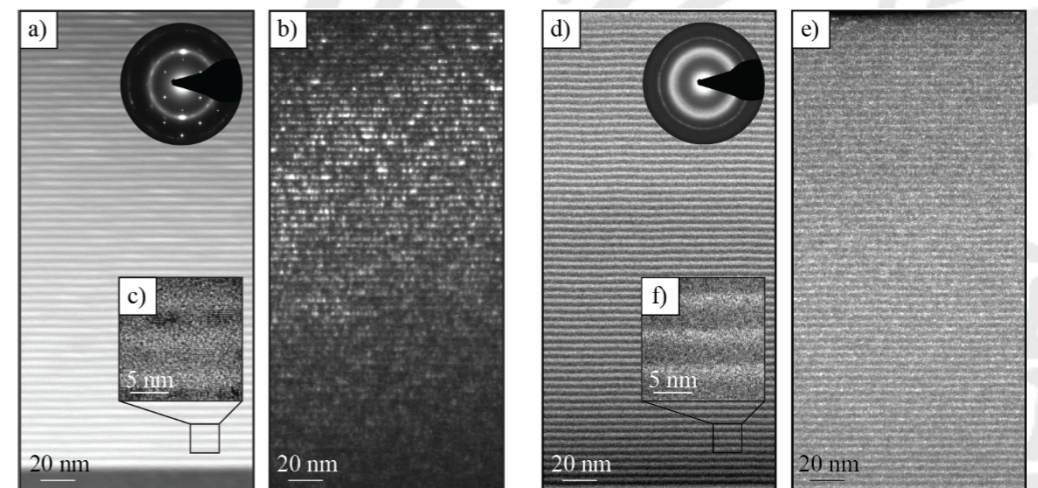
Silica spheres on silicon  
ACS Applied Materials & Interfaces **15**, 3772 (2023)



BornAgain model integrated into McStas

## Technical challenges/developments:

- Innovative optics (brilliance transfer)
- Focusing on sample/detector
- Detector technologies (count rate/dynamic range)
- Background suppression
- Polarisation – spin manipulation
- Focusing in momentum space



Ion assisted  $^{11}\text{B}_4\text{C}$  growth of NiTi super mirrors

# *The Swedish Instrument Project for Interface Science at ESS*

28 October 2021

*The*



# SAGGA

*The who sees everything*

*begins...*

[www.gisans.se](http://www.gisans.se)