SANS basics and SANS at ESS: LoKI

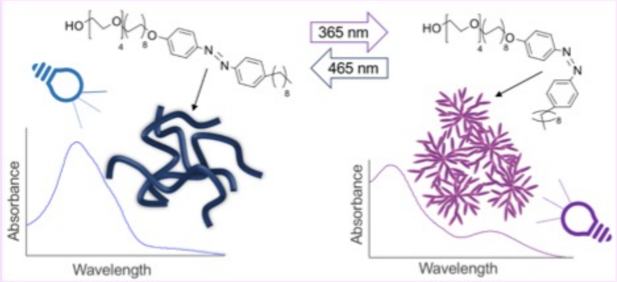
JUDITH HOUSTON
INSTRUMENT SCIENTIST - LOKI

25/04/2023

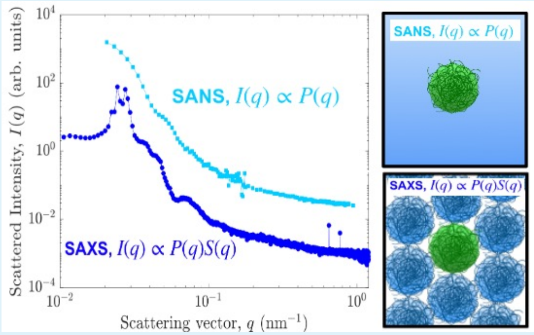
Who am I?

My Research Interests

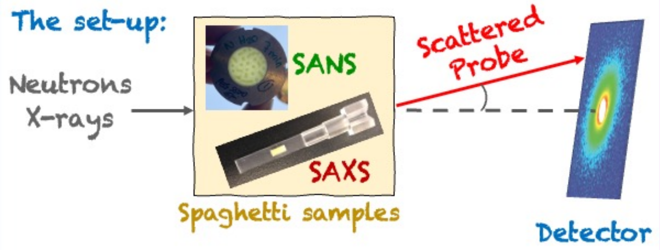
Self-assembled Systems
Conjugated polymers for OPVs
Proteins and surfactants for drug formulations
Photosurfactants



Nanogels
Probing the effect of softness of structure in bulk and at the interface



Food Science
Structural analysis of gluten versus gluten-free pasta

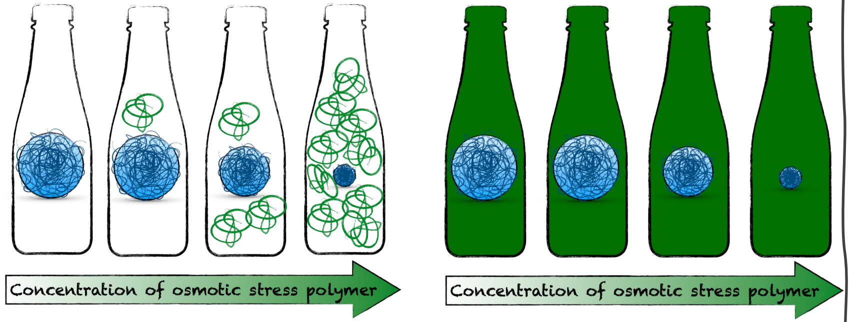


Current projects / collaborations

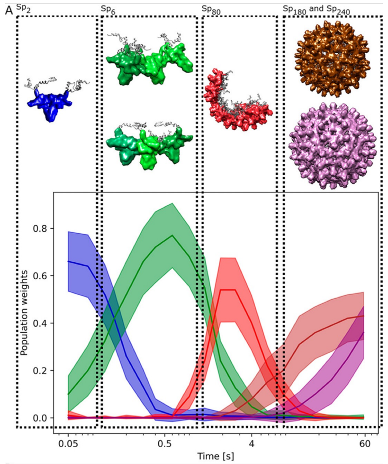
Nanogels with A. Scotti & W. Richtering (RWTH Aachen)

Probing softness with SANS

Science Advances, 2022, **8**, eabn6129
Soft Matter, 2022, **18**, 5750

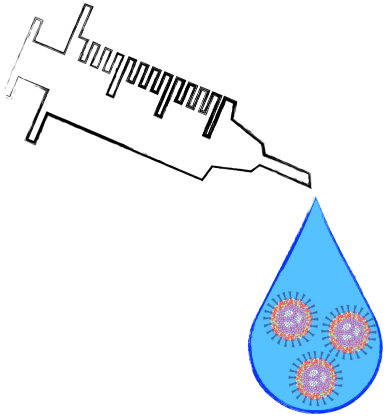


Viruses (W. Potrzebowski)



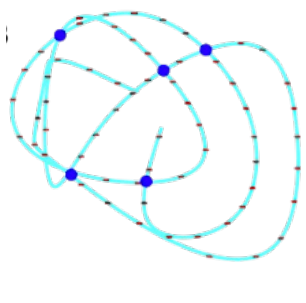
ILL beamtime upcoming

Lipid NPs (F. Sebastiani)



ISIS beamtime upcoming

Mucus balls (C. Garvey)



Proposal submitted

1

Small-angle neutron scattering

Why neutron scattering?

… natural tool for materials and technology research

What are neutrons?

Neutrons interact with the nuclei

- **Neutrons** interact with the **nuclei** of the atoms: **strong nuclear force**.
- Different to **light** and **X-rays,** which interact with **the electron clouds** surrounding the nuclei: **electromagnetic force**.

- We can imagine the **nucleus** of the size of a **marble**.

What are neutrons?

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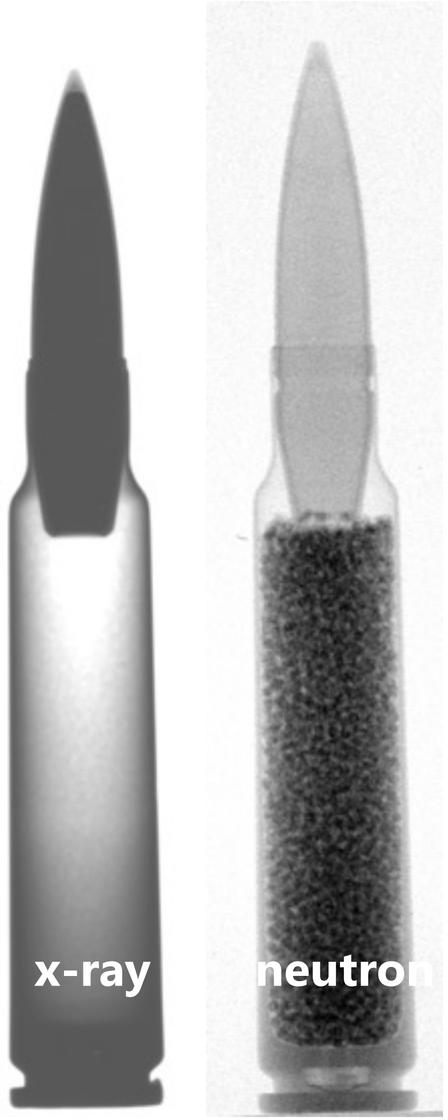
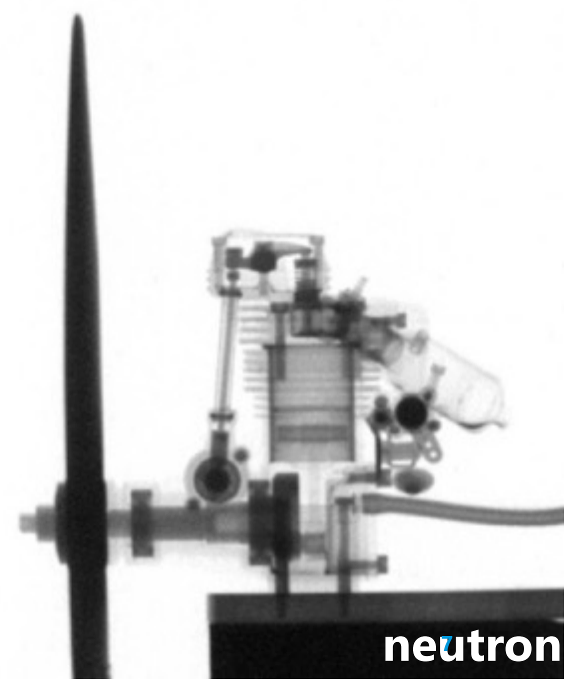
- We can imagine the **nucleus** of the size of a **marble**.
- The **atom** in proportion will be as big as a football **stadium**.
- **Neutrons interact** with the sample **only** when they **hit the nucleus**.

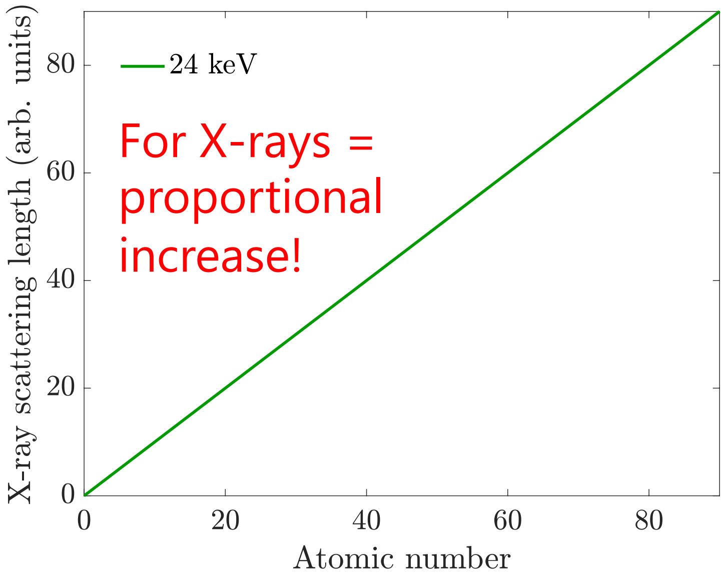
X-rays and neutrons see things differently

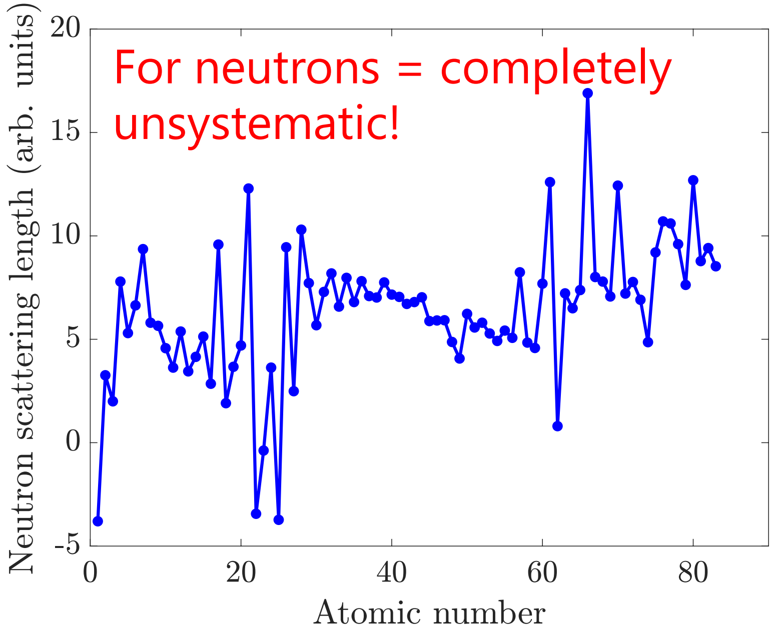


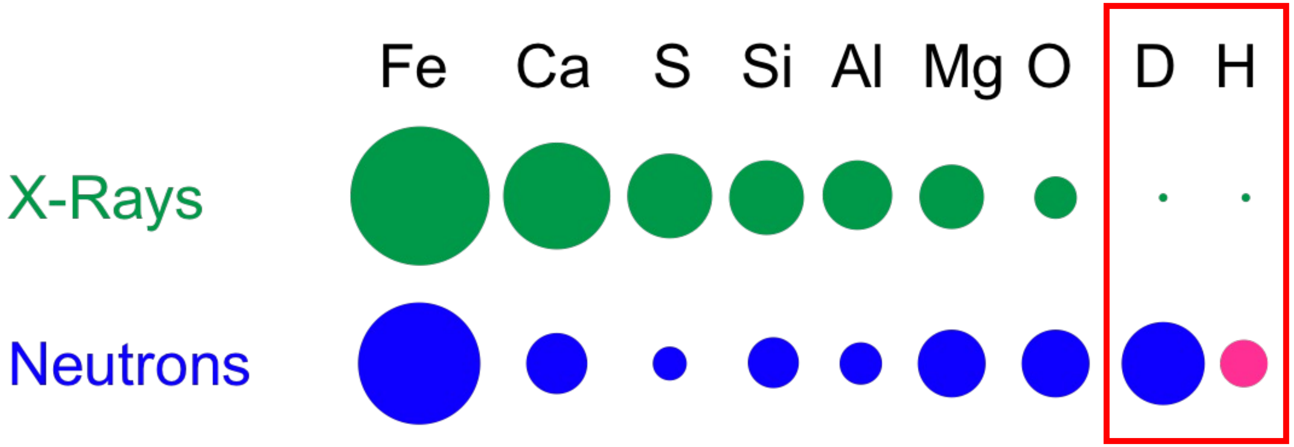


Courtesy of the NIAG group, PSI, Switzerland.

X-rays and neutrons

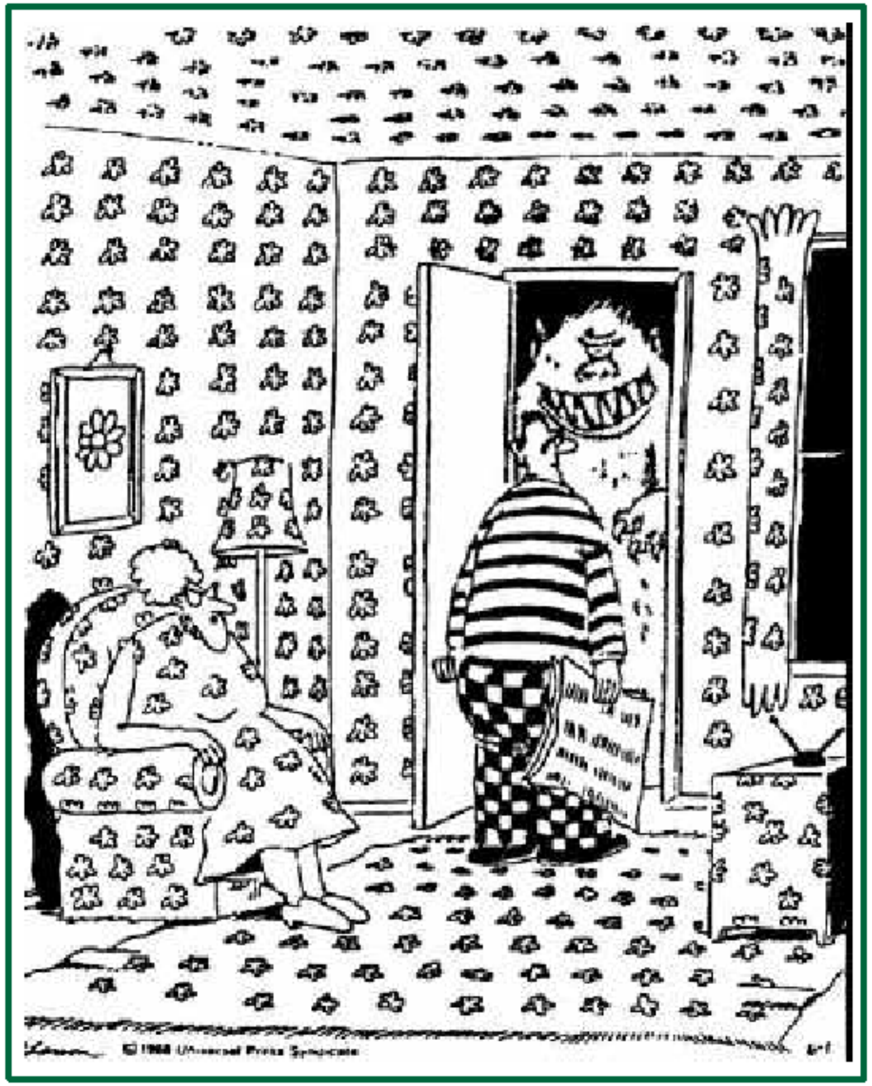






...even for different isotopes of the same element!

Neutrons and contrast matching



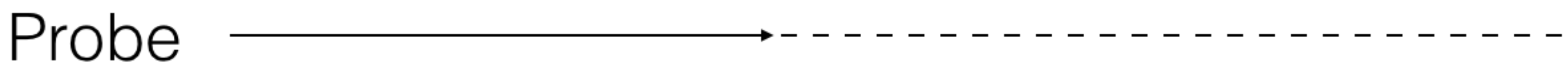
When the monster came, Lola remained undetected.

Harold, of course, was immediately devoured.

This same principle can be applied to study our samples!

Small-angle scattering

Experimental technique which uses **elastic scattering** at **small angles** to investigate the structure of substances at a mesoscopic scale of ~1–200 nm



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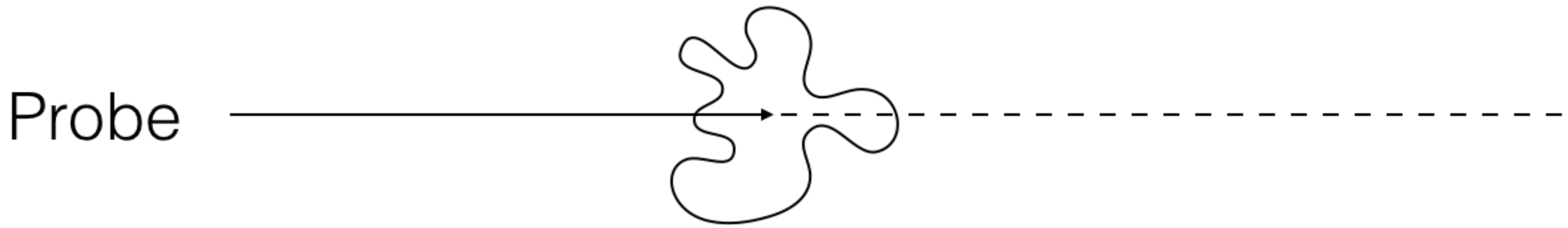

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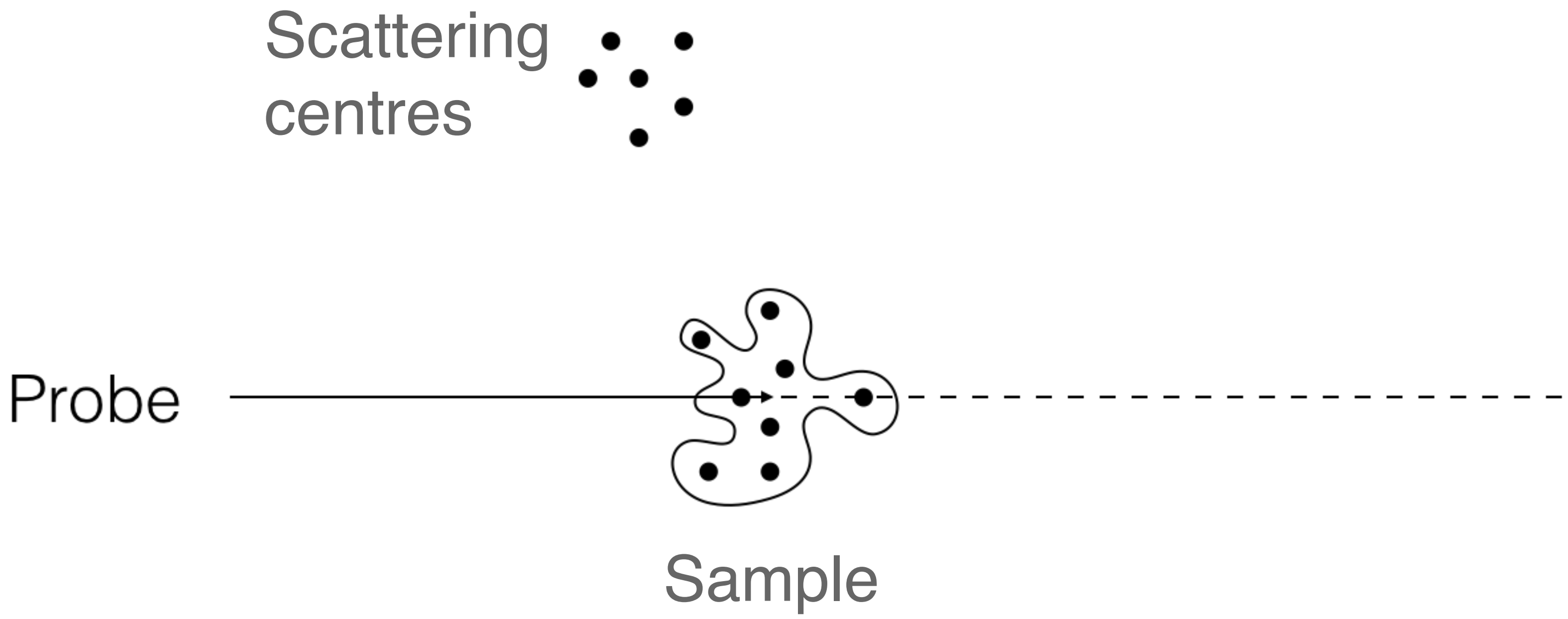

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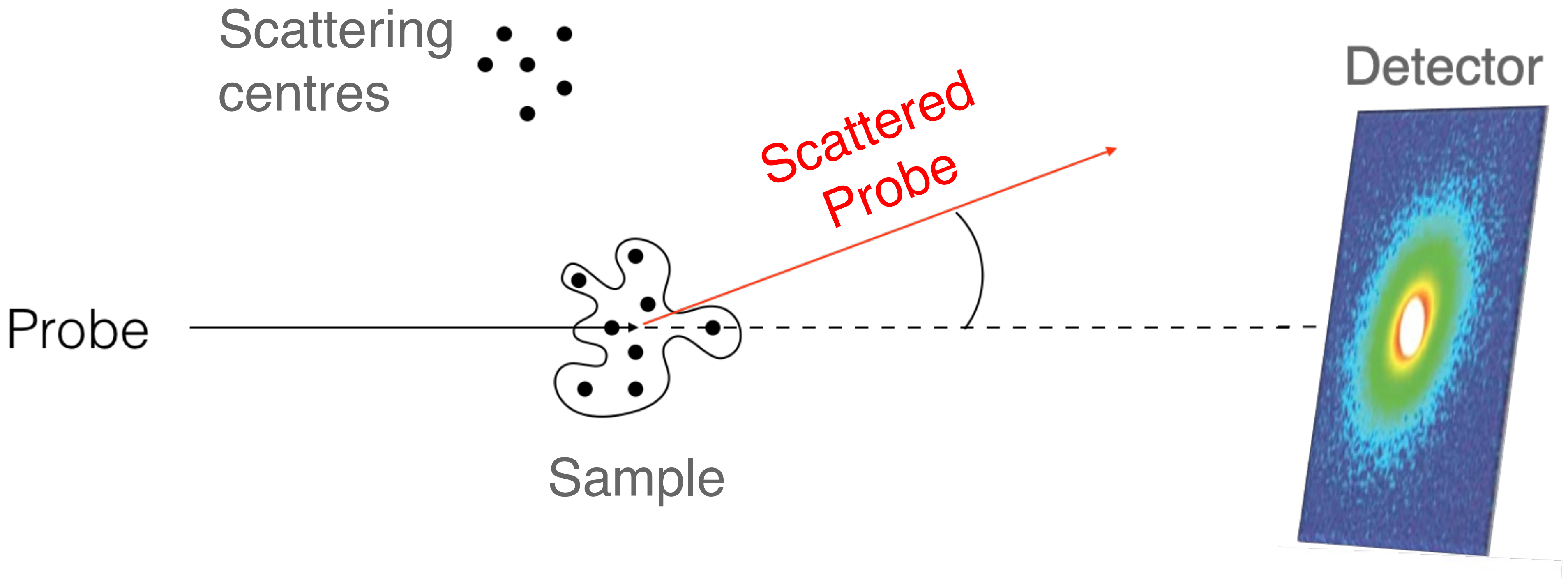


Scattering from a nucleus: scattering vector

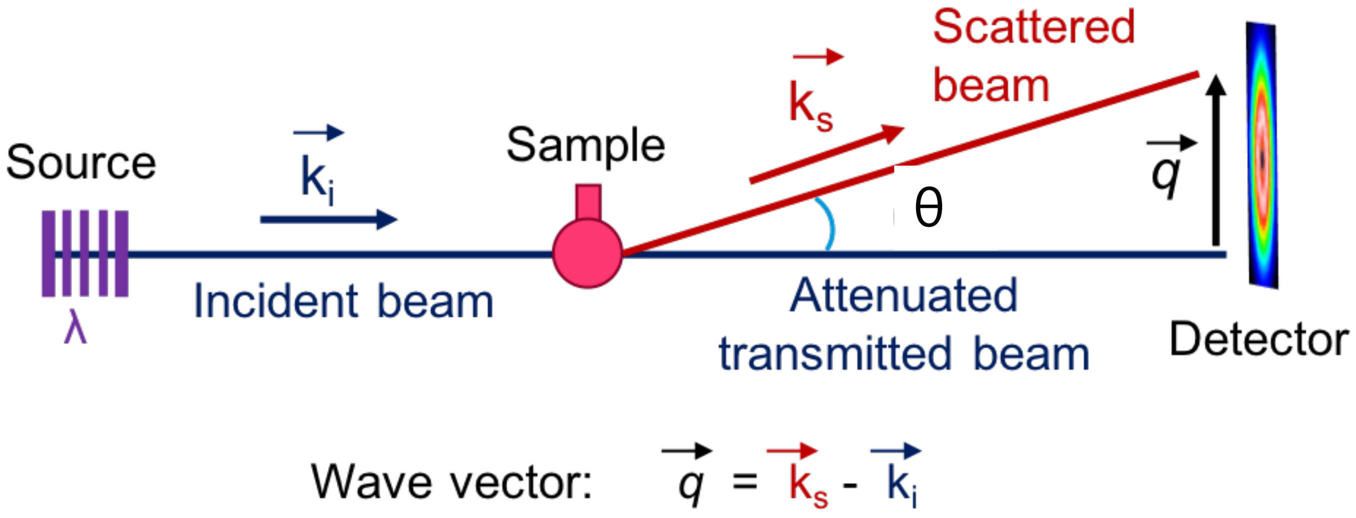
Consider scattering geometry & Bragg's law:

$$\lambda = 2d sin(\frac{\theta}{2})$$

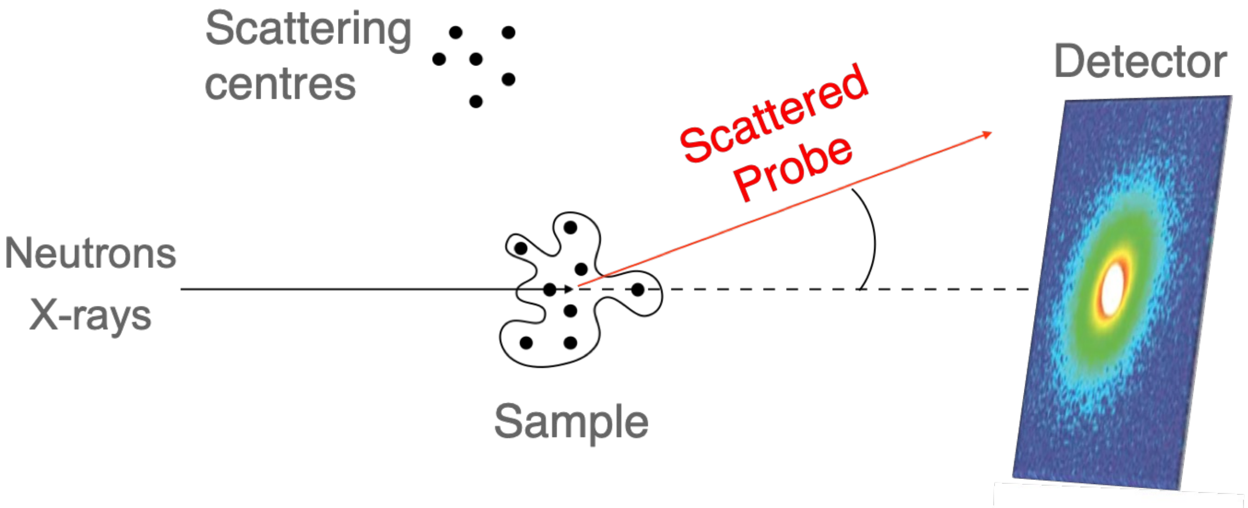
Switch to reciprocal space:

$$q = \frac{2\pi}{d}$$

$$q = \frac{4\pi}{\lambda} sin(\frac{\theta}{2})$$



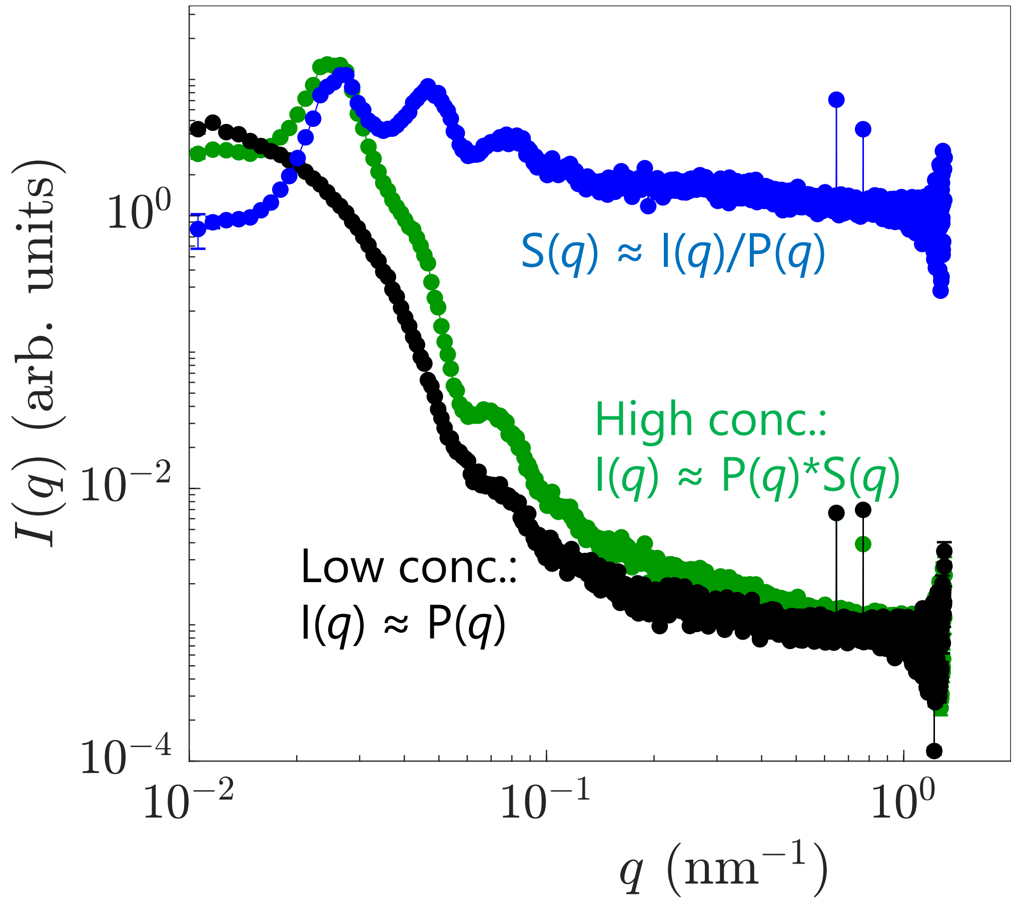
Small-angle scattering



$$I_{exp}(q) = n\Delta\rho^2 V^2 P(q) S(q)$$

Form factor: Shape, size

Structure factor: Arrangement



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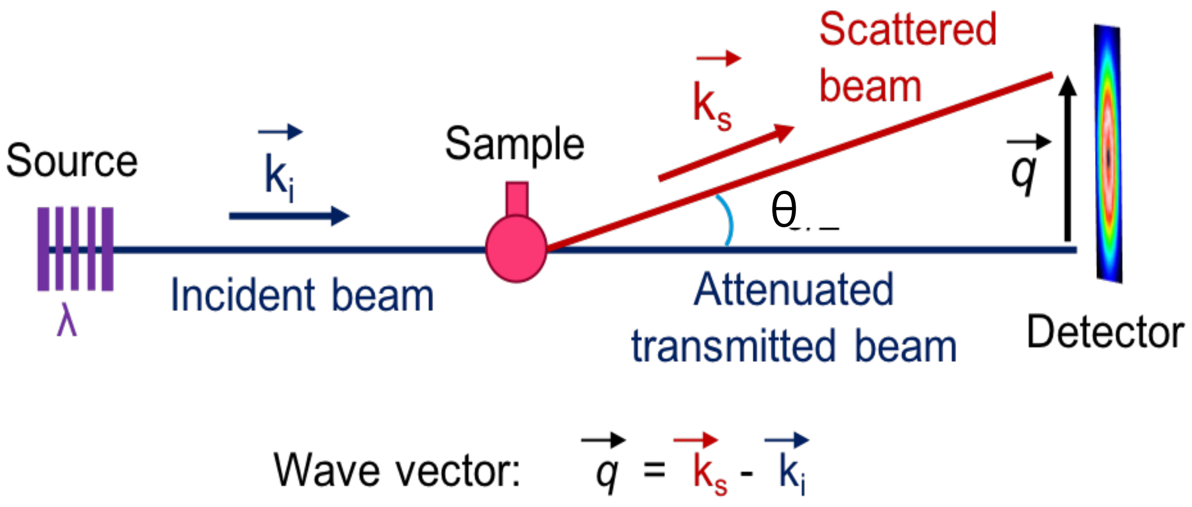

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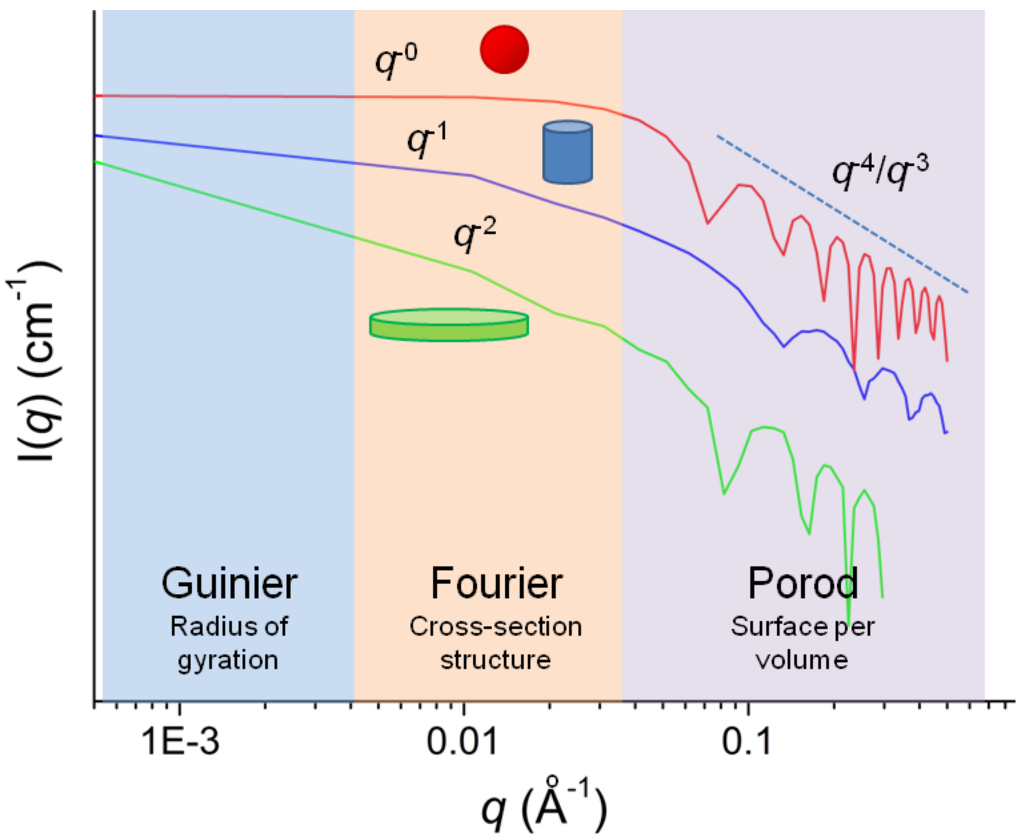


Continuous vs. time-of flight

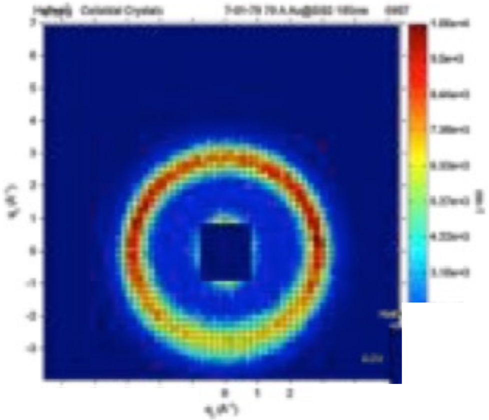
$$q = \frac{4\pi}{\lambda} sin(\frac{\theta}{2})$$

We need to determine the wavevector, Q….

Continuous
Fixed wavelength (monochromatic)
Fixed λ, varying θ
Need several measurements at different detector distances to cover adequate q-range
Typically reactor sources (exceptions: TOF instruments in monochromatic mode)

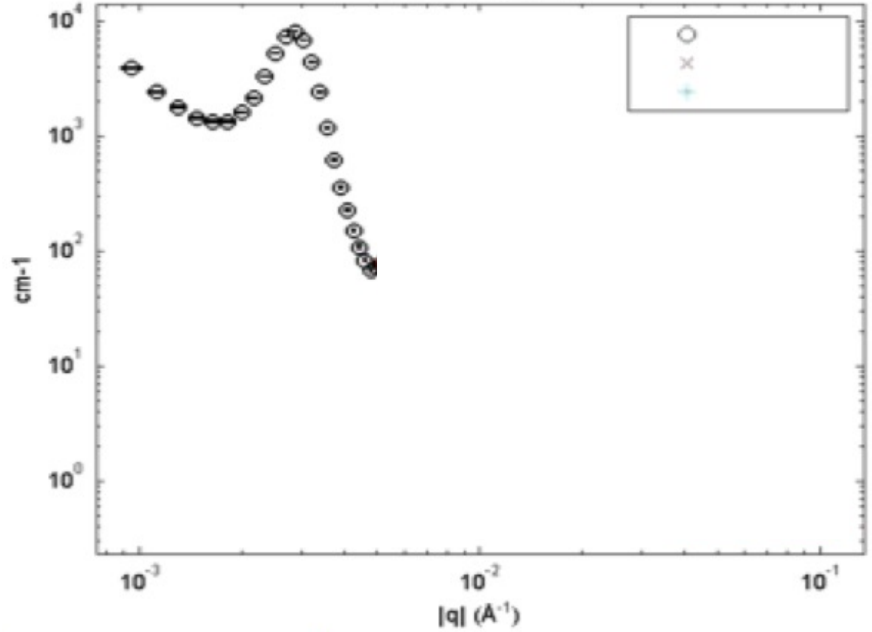
Continuous vs. time-of flight

Need several measurements at different distances to cover an adequate *Q*-range



Low q:
Largest sample-to-detector distance

Monochromatic beam



Figures from ILL

Continuous vs. time-of flight

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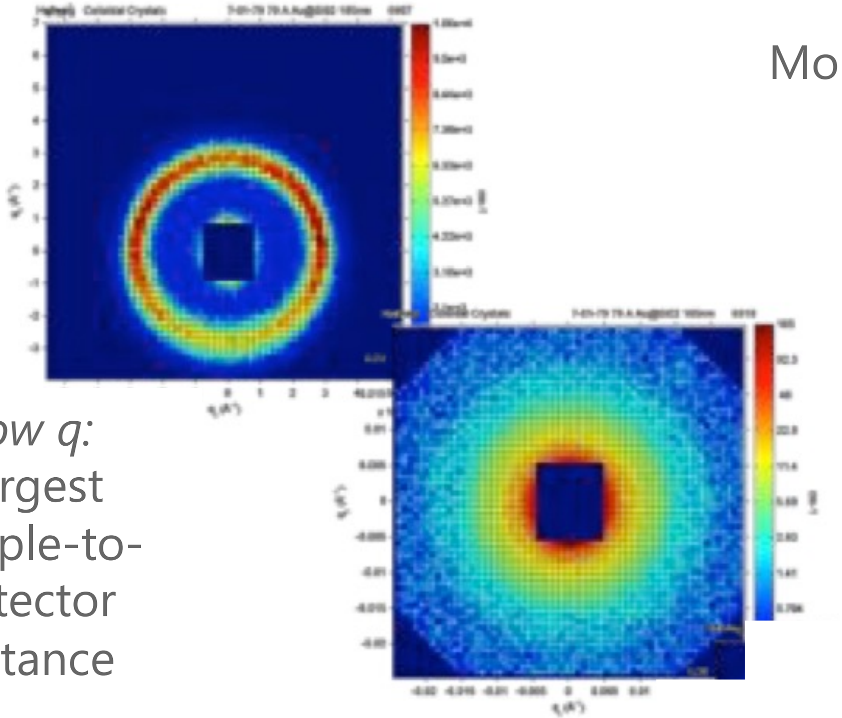

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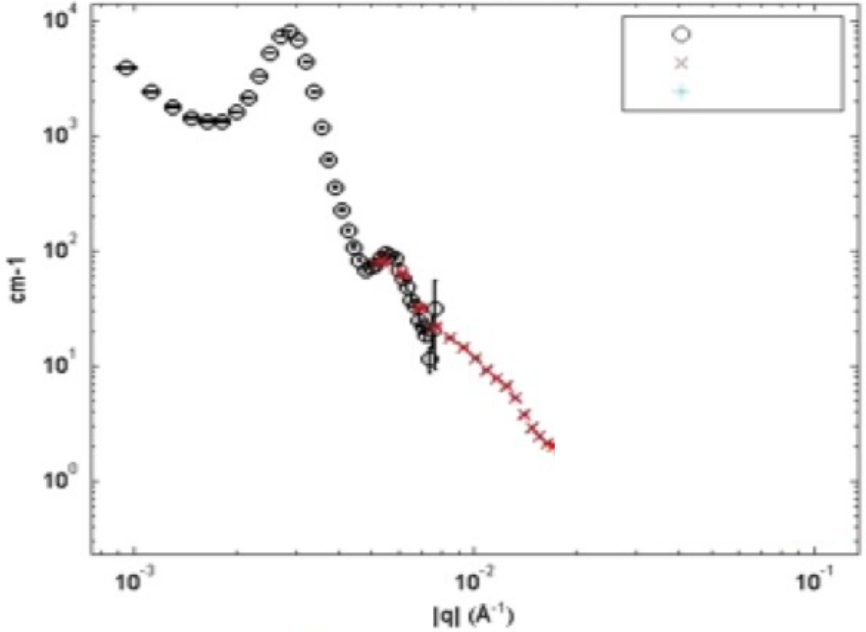
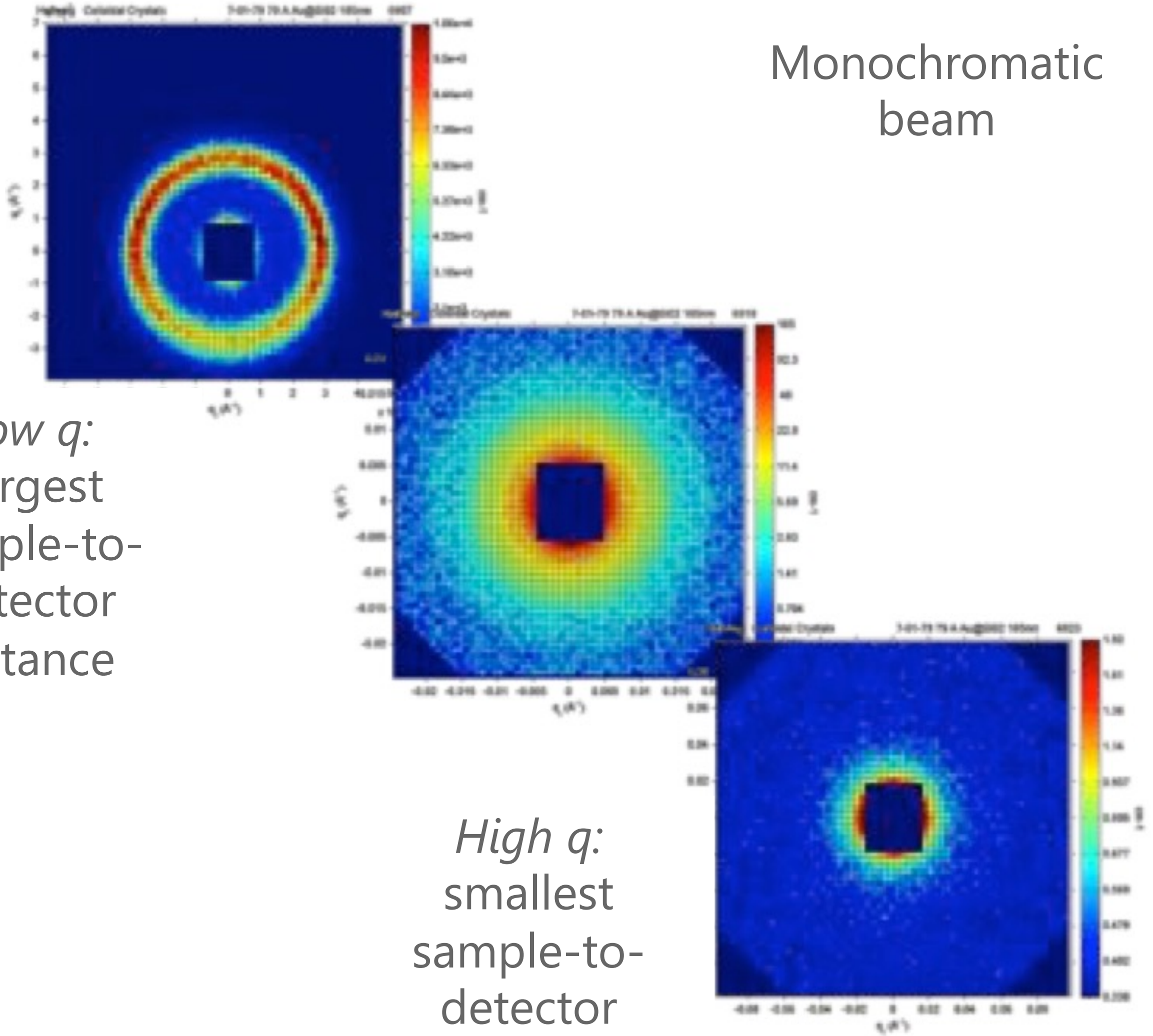


Figures from ILL

Continuous vs. time-of flight

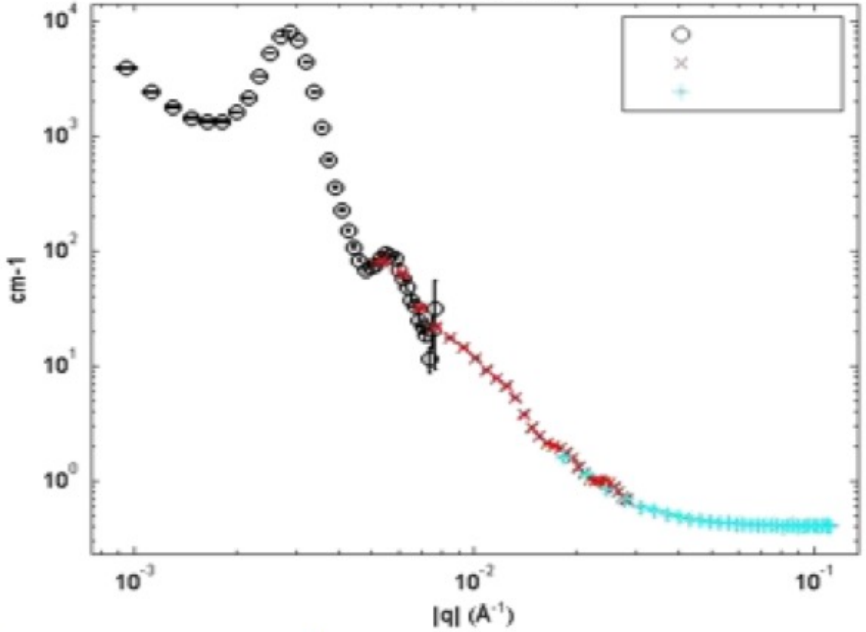
Need several measurements at different distances to cover an adequate *Q*-range

Monochromatic beam



Low q: Largest sample-to-detector distance

High q: smallest sample-to-detector distance



Figures from ILL

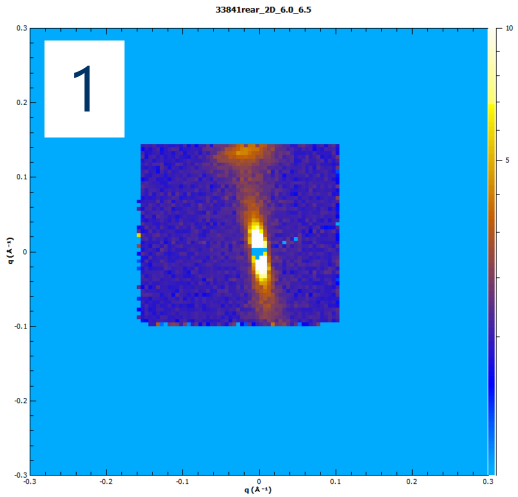
Continuous vs. time-of flight

$$q = \frac{4\pi}{\lambda} sin(\frac{\theta}{2})$$

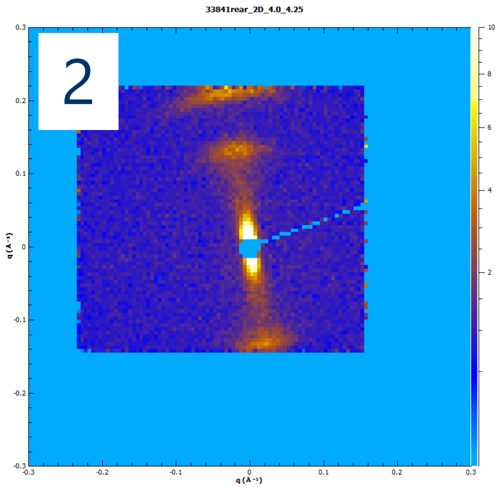
We need to determine the wavevector, Q….

Continuous	Time-of-flight
Fixed wavelength (monochromatic)	Wavelength band
Fixed λ, varying θ	Varying θ, varying λ
Need several measurements at different detector distances to cover adequate q-range	Large dynamic q-range at one detector distance, q_{max}/q_{min}
Typically reactor sources (exceptions: TOF instruments in monochromatic mode)	Typically spallation sources (exceptions: ILL D33 and ANSTO Bilby)

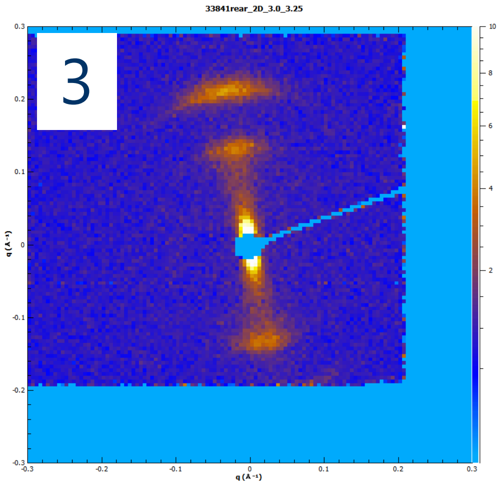
Continuous vs. time-of flight



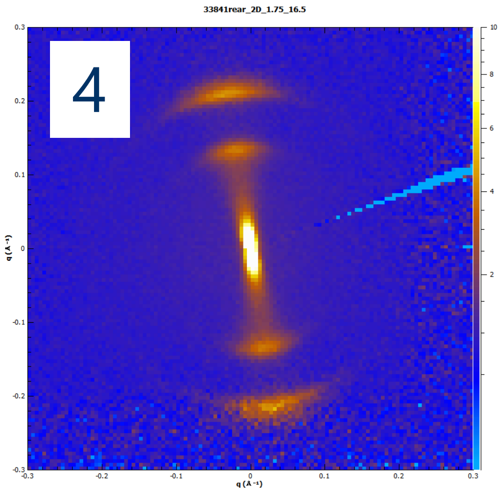
"fixed wavelength"
~6.25 Ǻ



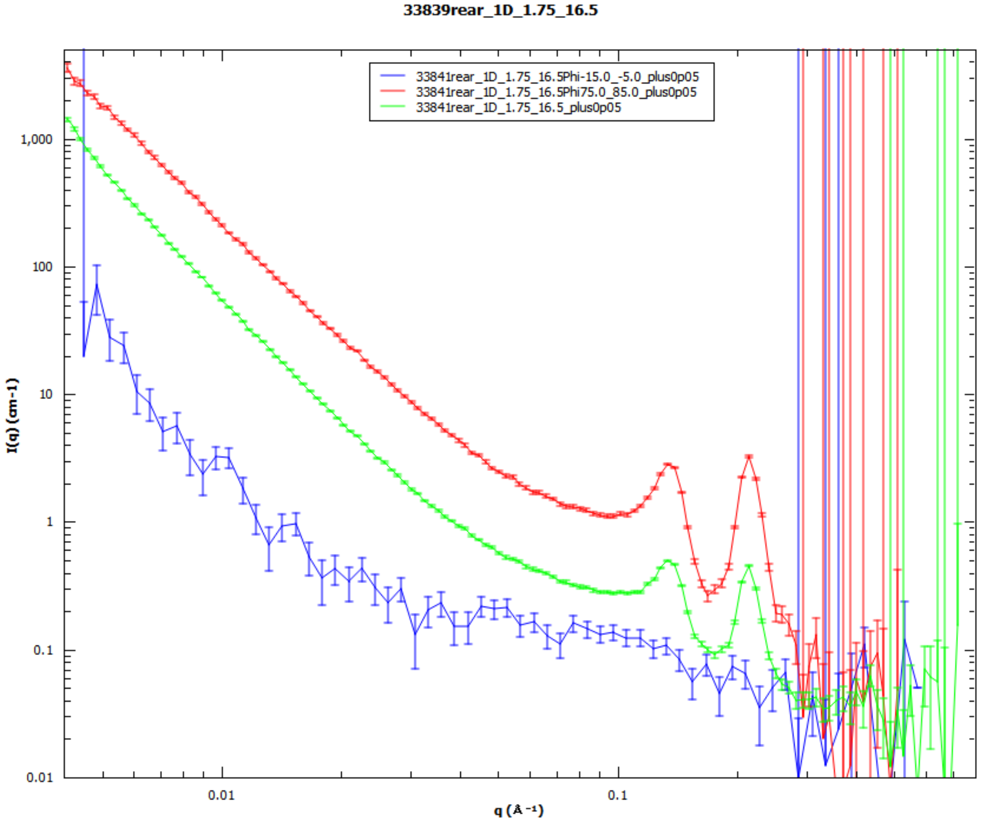
Shorter wavelengths
expand Qmax



Even shorter wavelengths
expand Qmax further

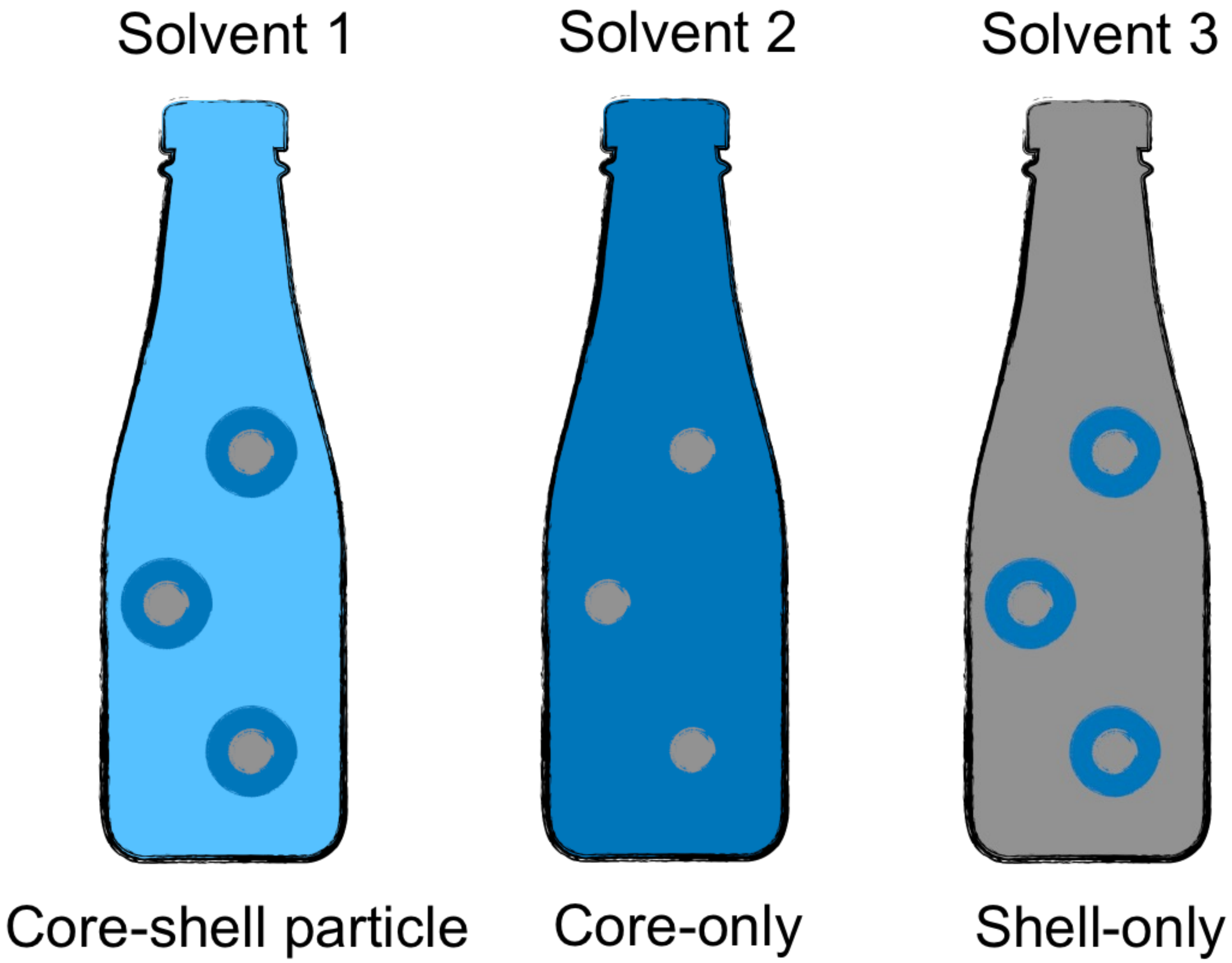


Full 1.75 to 16.5 Å gives a
wide simultaneous Q range.



Courtesy of R. K. Heenan and M. Hollamby

Neutrons and contrast matching

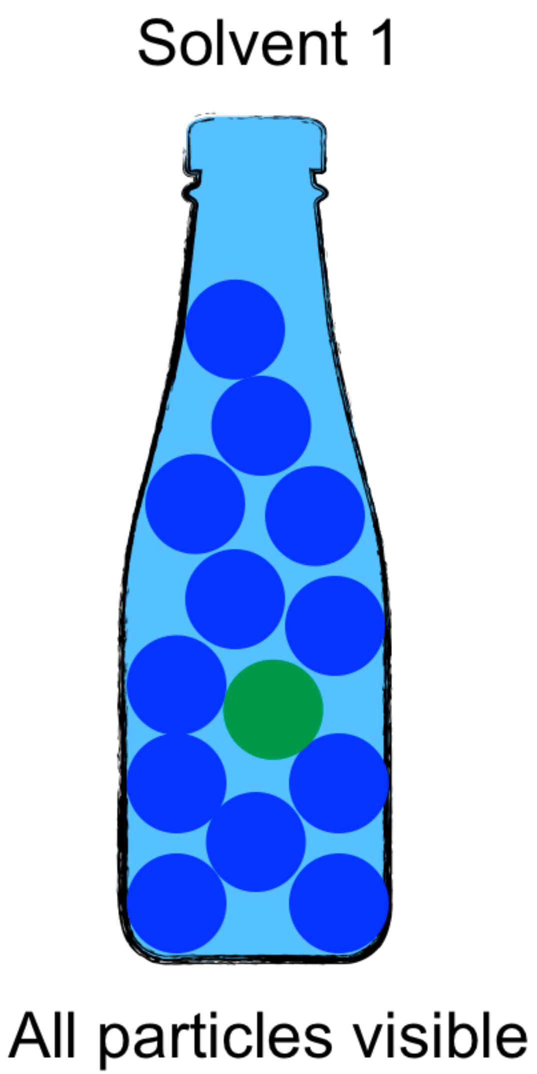


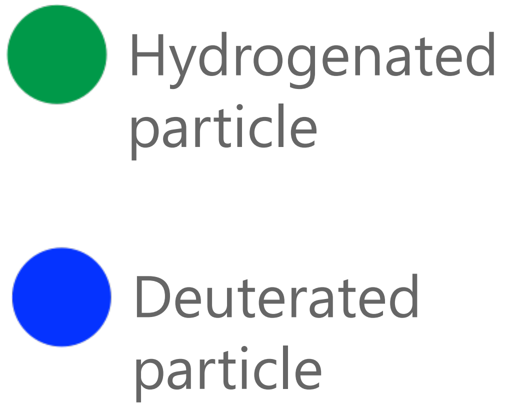
$$I_{exp}(q) = n\Delta\rho^2 V^2 P(q) S(q)$$

Selective deuteration in combination with neutrons lets us investigate selected parts of complex assemblies.

Combining X-Ray and Neutron measurements provides more information

Example: microgels in crowded environment





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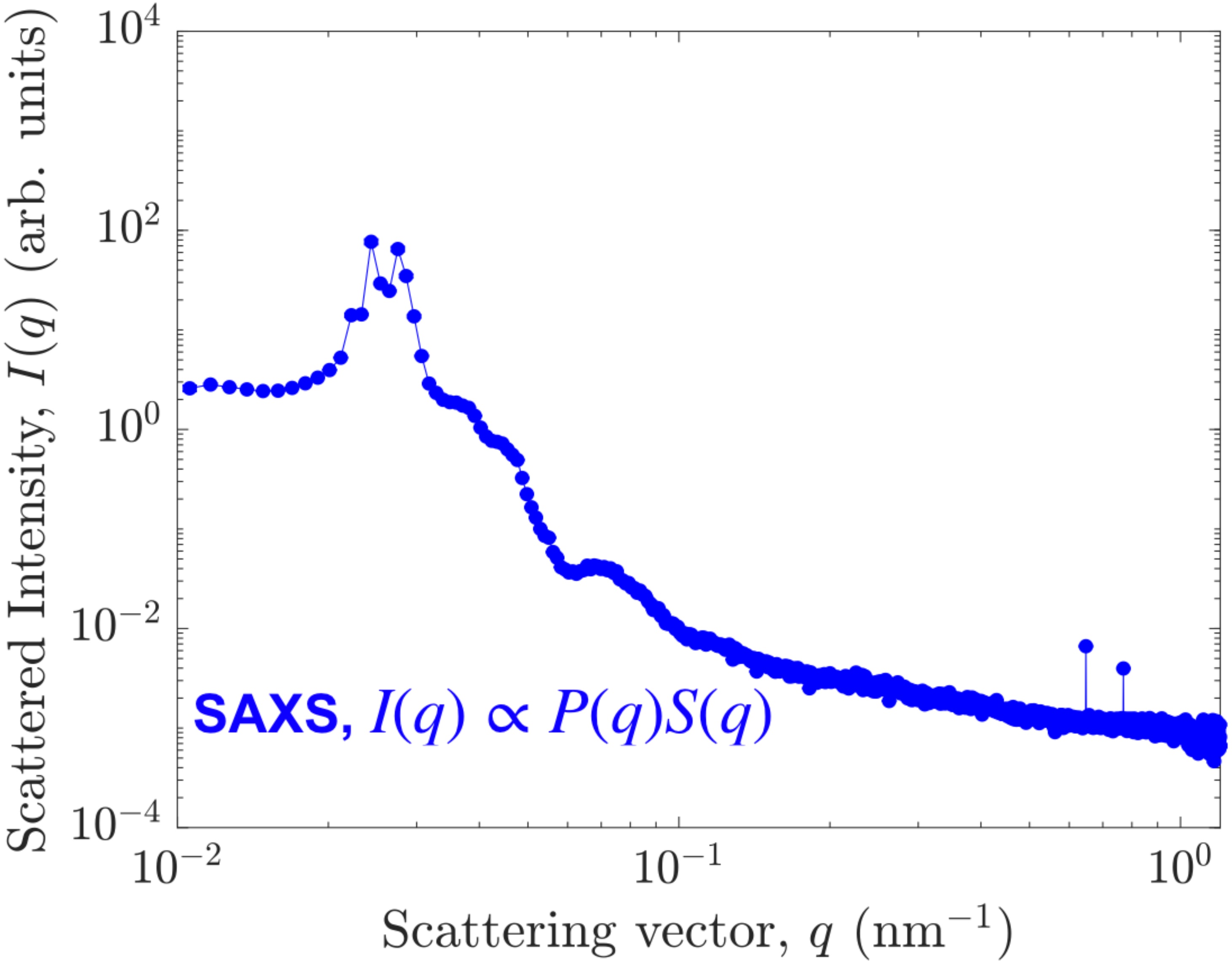
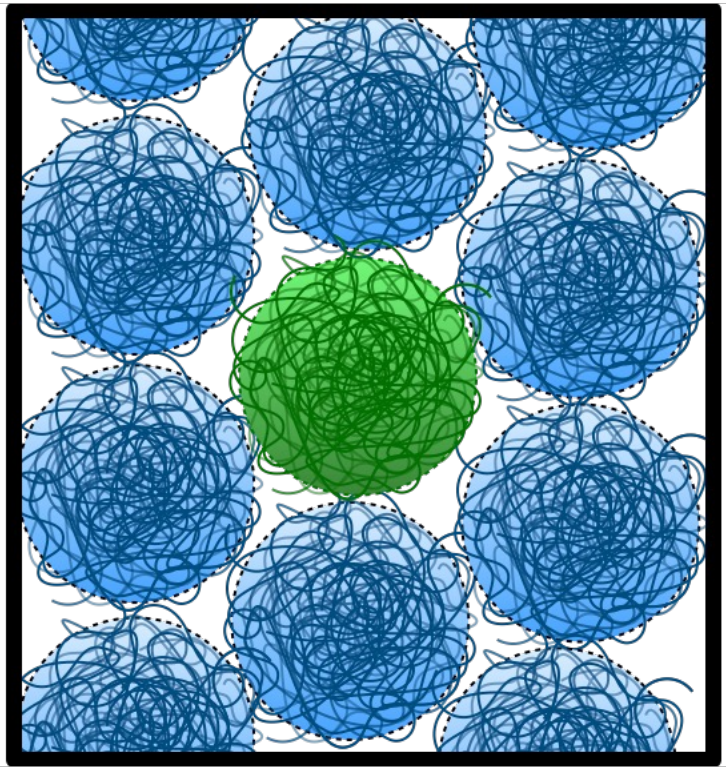
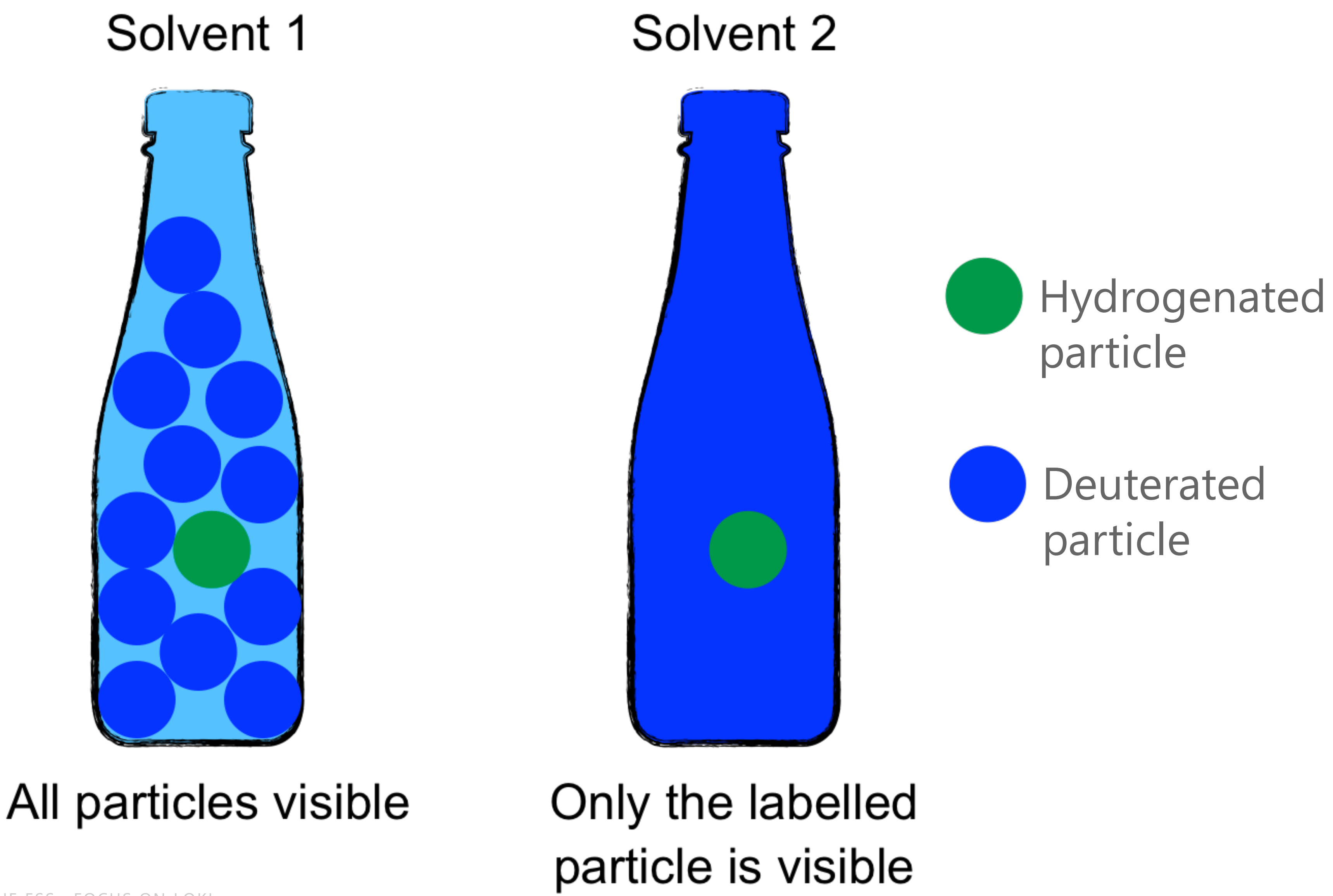




Courtesy of Andrea Scotti (RWTH)

Example: microgels in crowded environment



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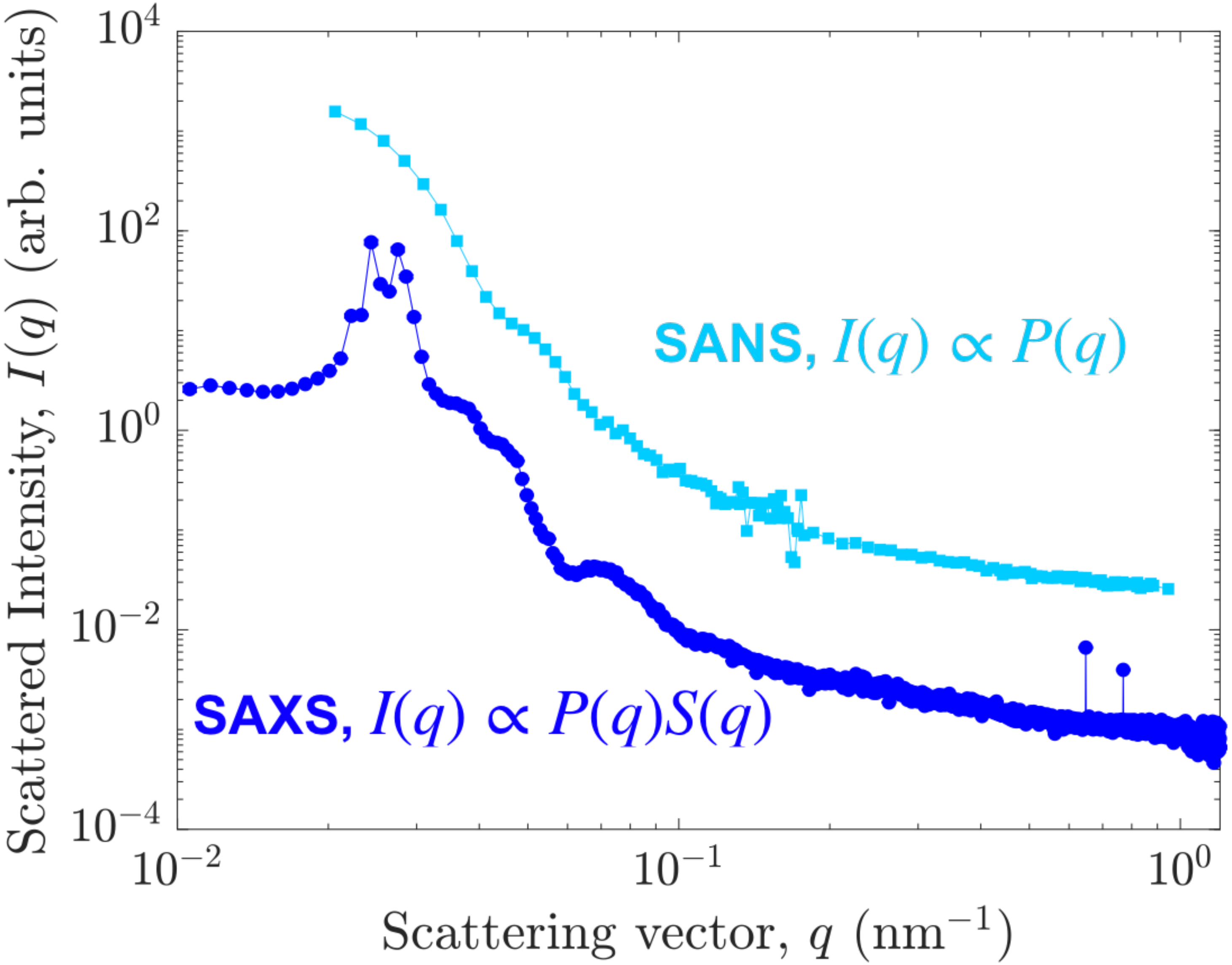
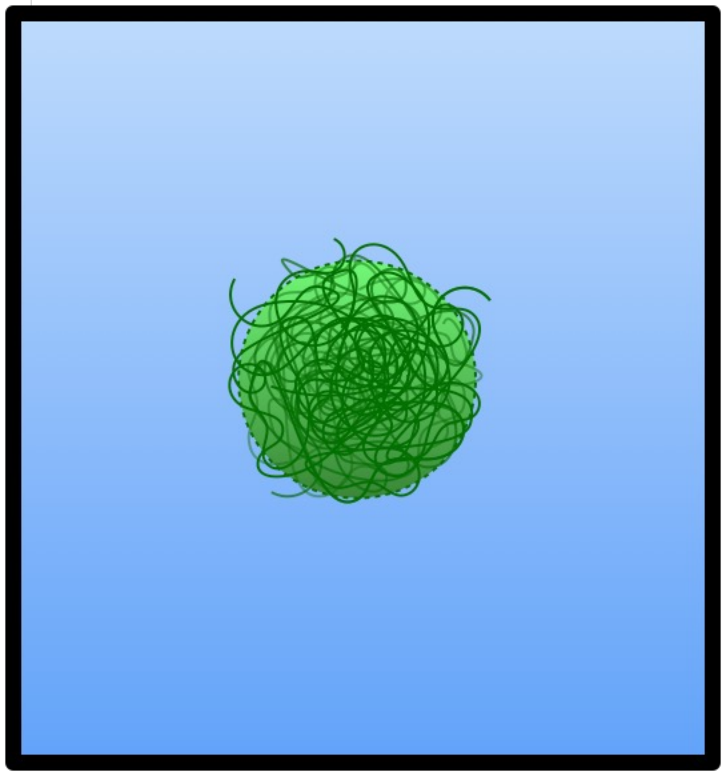


SANS, $I(q) \propto P(q)$

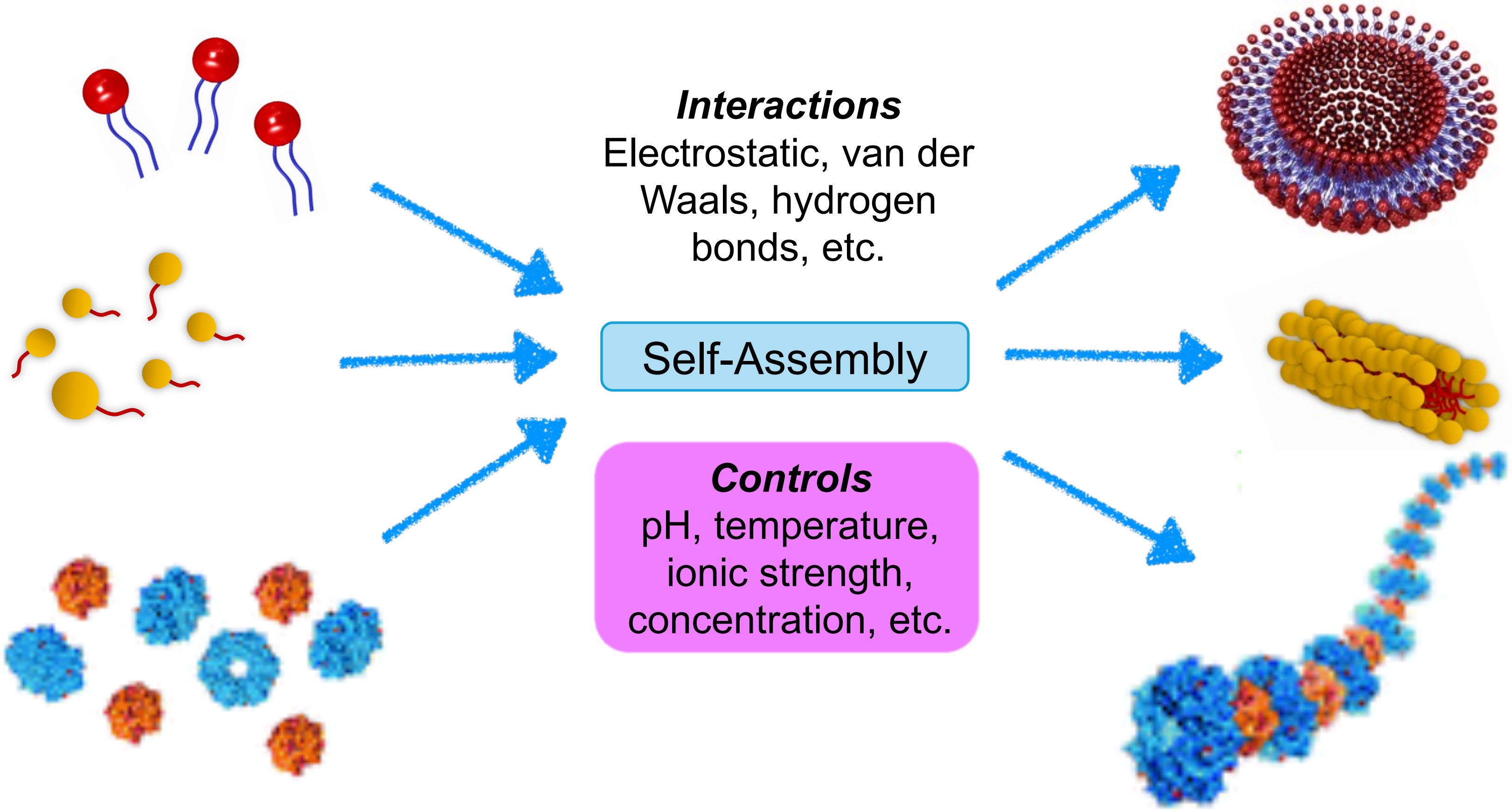


Courtesy of Andrea Scotti (RWTH)

2

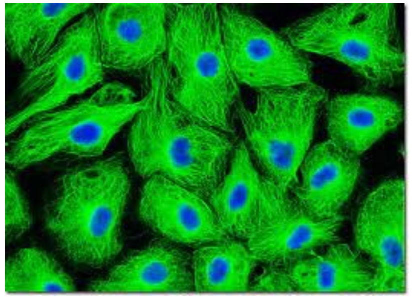
What can we study with SANS?

Self-assembly



Motivation

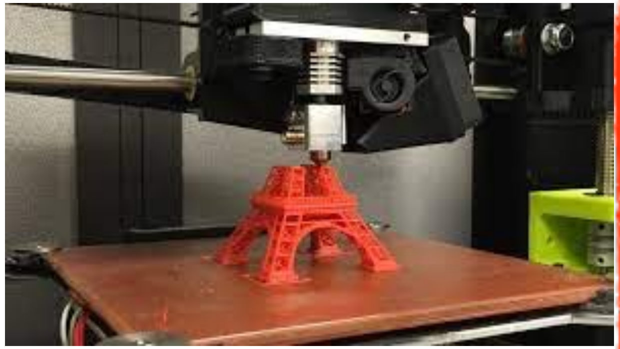
Biological materials



Soft Matter: Materials with properties between **liquids** and **solids**

Foams

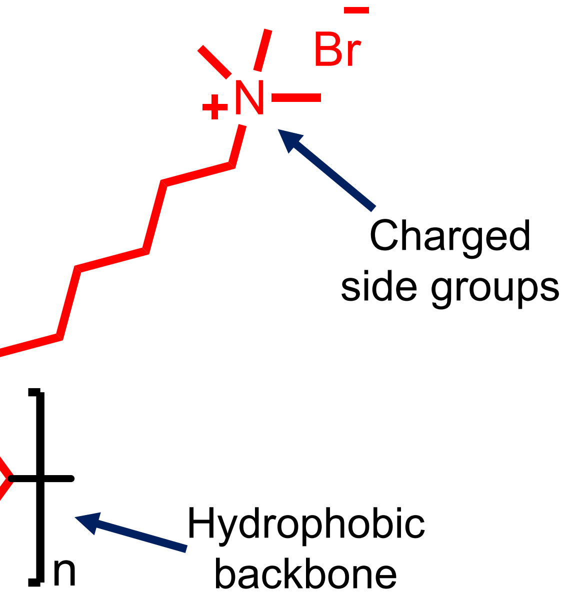
Polymers

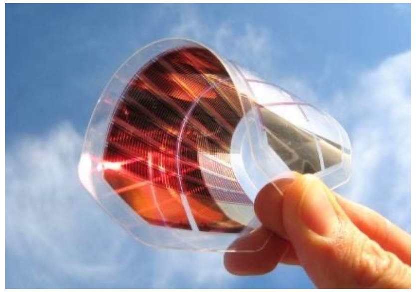


Colloidal suspensions

Liquid crystals

Targeted energy materials





π-conjugated hydrophobic backbone controls optical and electronic properties.

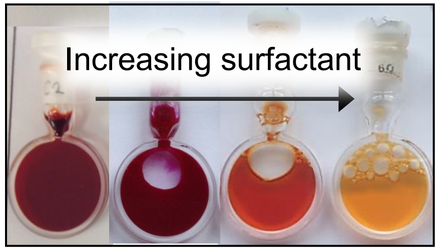
Side-chains control solubility, aggregation and self-assembly.

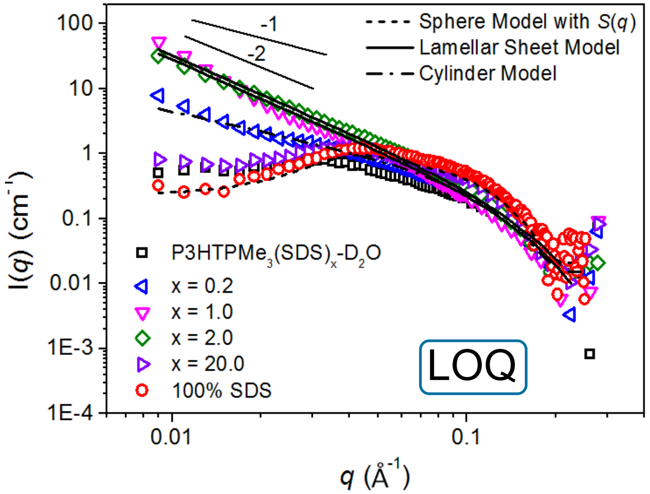
Block copolymers facilitate tuning of properties.

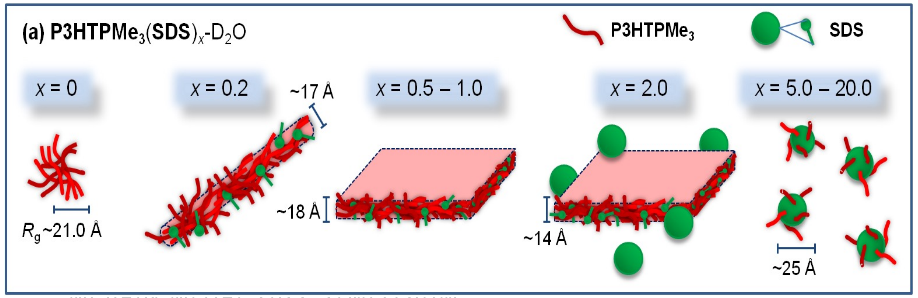
Device performance depends on the inherently-linked **optoelectronic properties** and **nanoscale morphology** of the polymer

Targeted energy materials

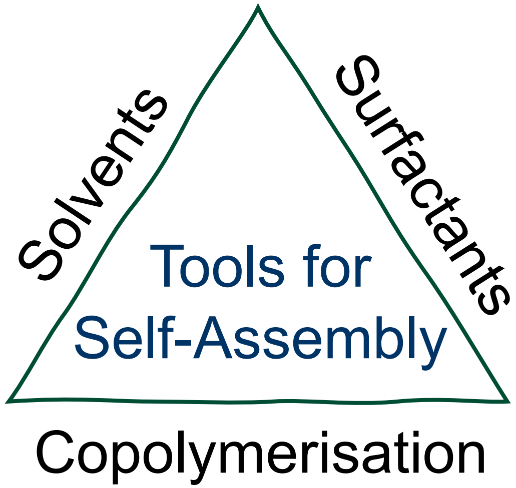
Self-Assembly in Solution



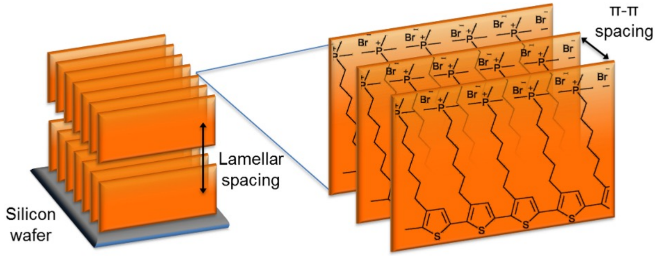


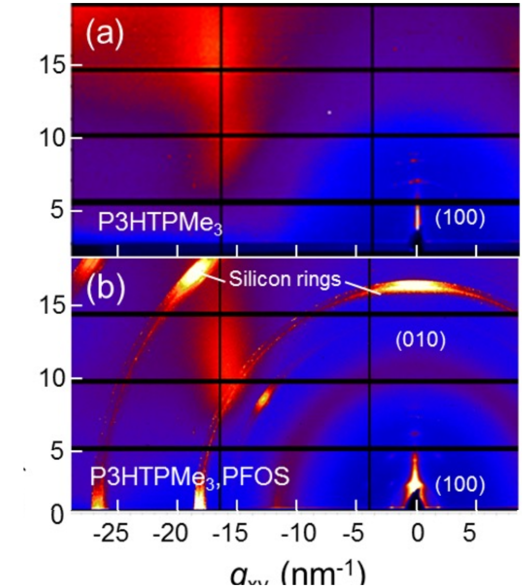


Nanoscale, 2017, **9**, 17481
Polym. Chem., 2014, **5**, 3352
J. Mater. Chem. A, 2015, **3**, 23905



Self-Assembly in Thin Films

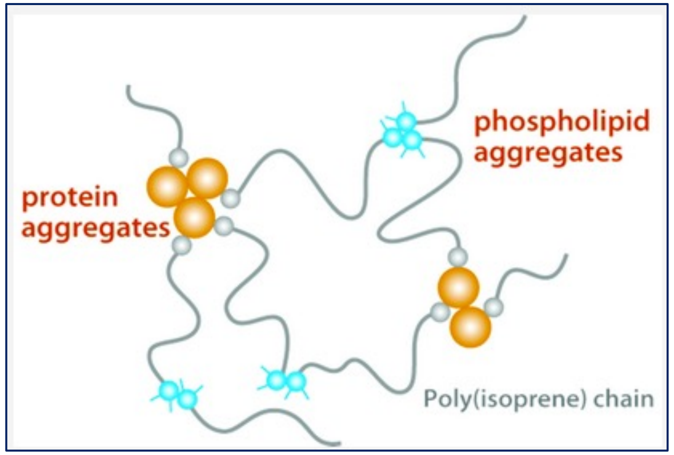




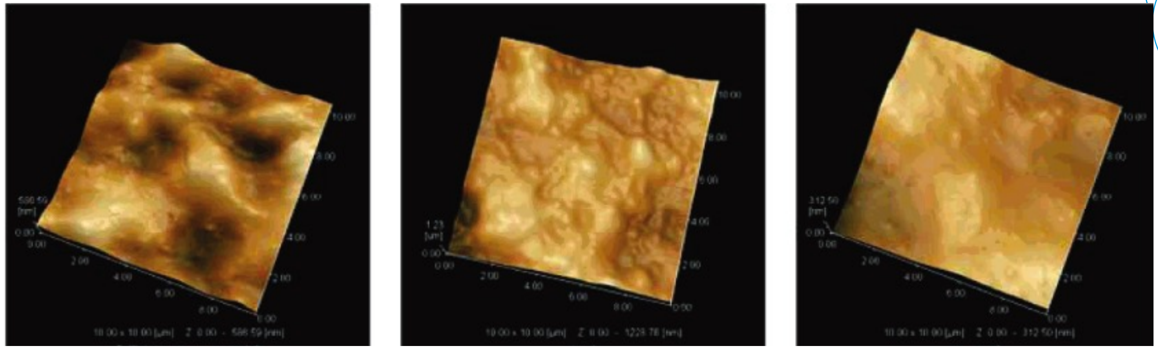
- Crystalline regions: improved charge generation;
- Amorphous regions: enhance charge transport;
- Orientation of polymer chains: Impacts energy level alignment.

SANS

e.g. natural *vs.* synthetic rubber



Atomic force micrographs

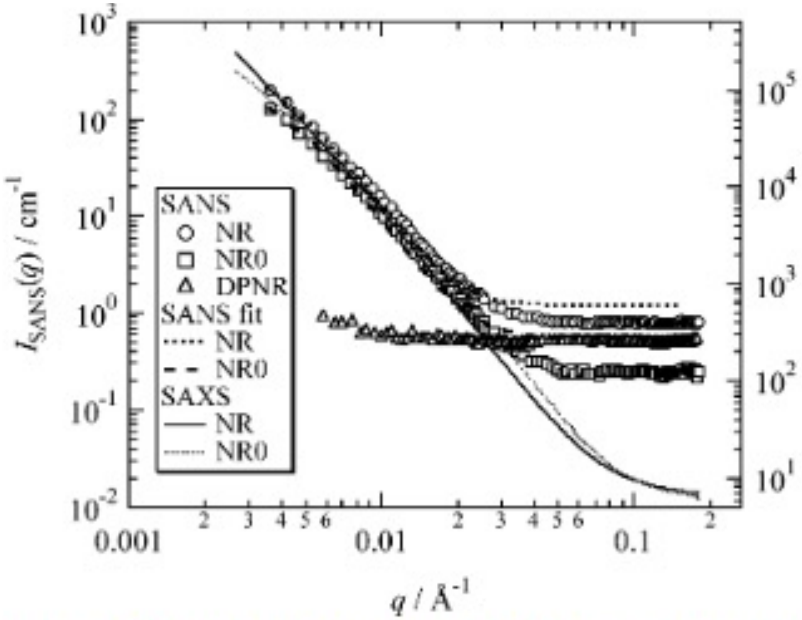


Natural rubber

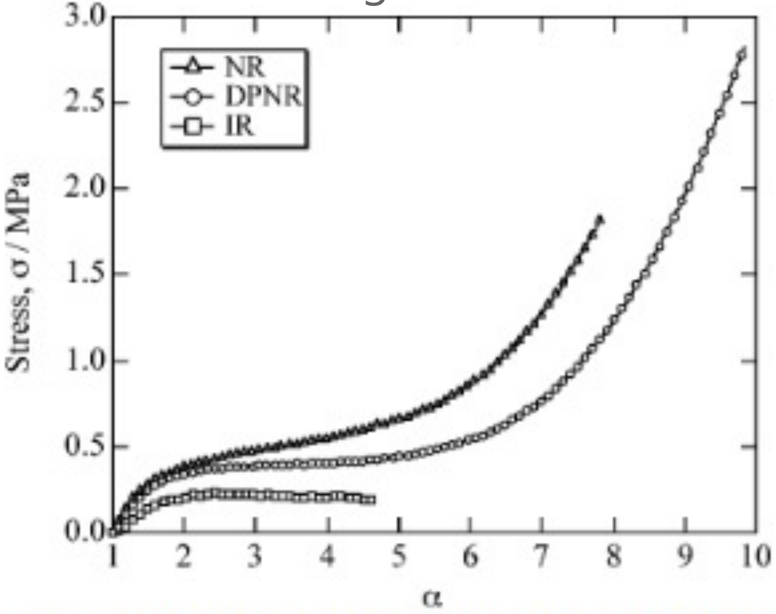
Deproteinized-natural rubber

Synthetic isoprene rubber

SANS & SAXS



Stress-elongation ratio curves



Inhomogenities in natural rubber due to phospholipid rather than protein aggregates, imparting on them their superior mechanical strength

Karino *et al.*, *Biomacromolecules*, 2007, **8**, 693-699

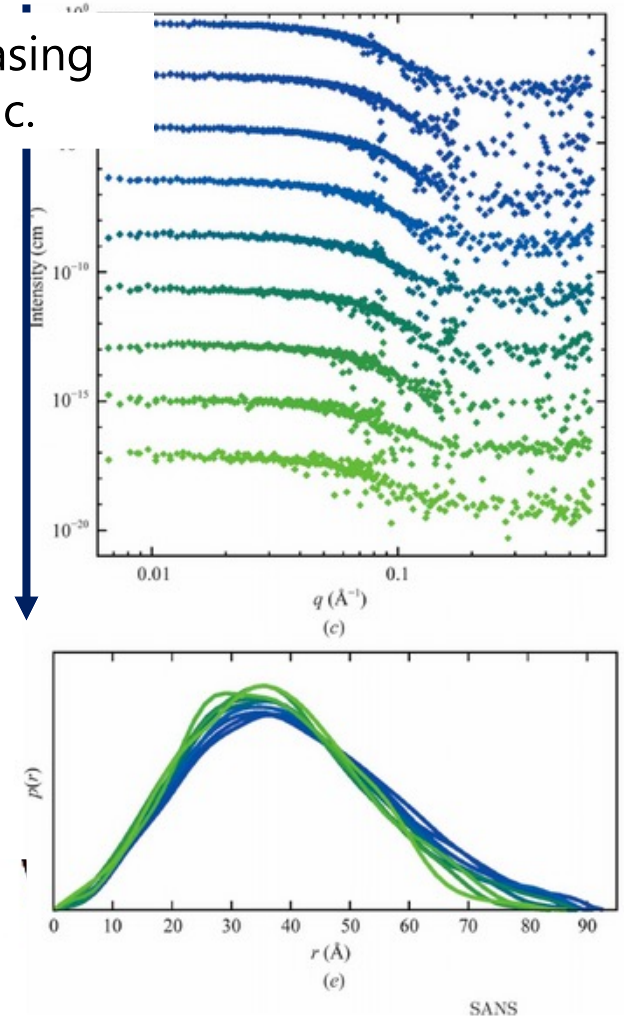
Size-exclusion chromatography SANS

e.g. phospholipid bilayer nanodiscs

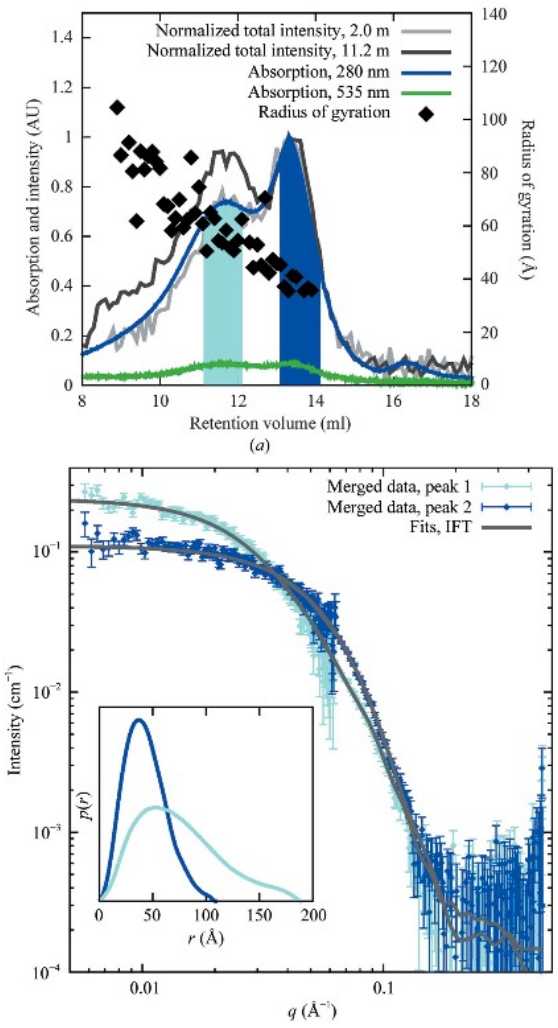
Challenge:
Obtaining SAS data on monodisperse complex biological structures is often challenging owing to sample degradation and/or aggregation

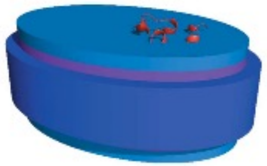
Bare phospholipid nanodisc

decreasing conc.



Protein-loaded phospholipid nanodisc





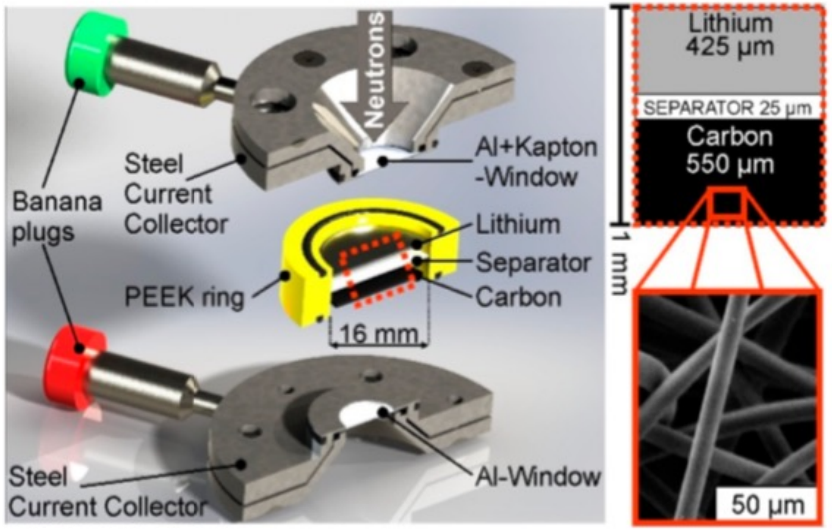
Johansen *et al.*, *Acta Cryst.*, 2018, **D74**, 1178-1191

In situ analysis of batteries and fuel cells

The combination of **impedance spectroscopy** and **SANS** yields valuable insights into the precipitation and dissolution of lithium sulfide during 10 cycles of galvanostatic cycling of a battery.

Deuterated electrolyte **increases strongly the sensitivity** to detect the sulfur and Li_2S precipitates at the carbon host electrode and allows the time-dependent initial wetting of the system to be observed.

Battery cell for SANS measurements



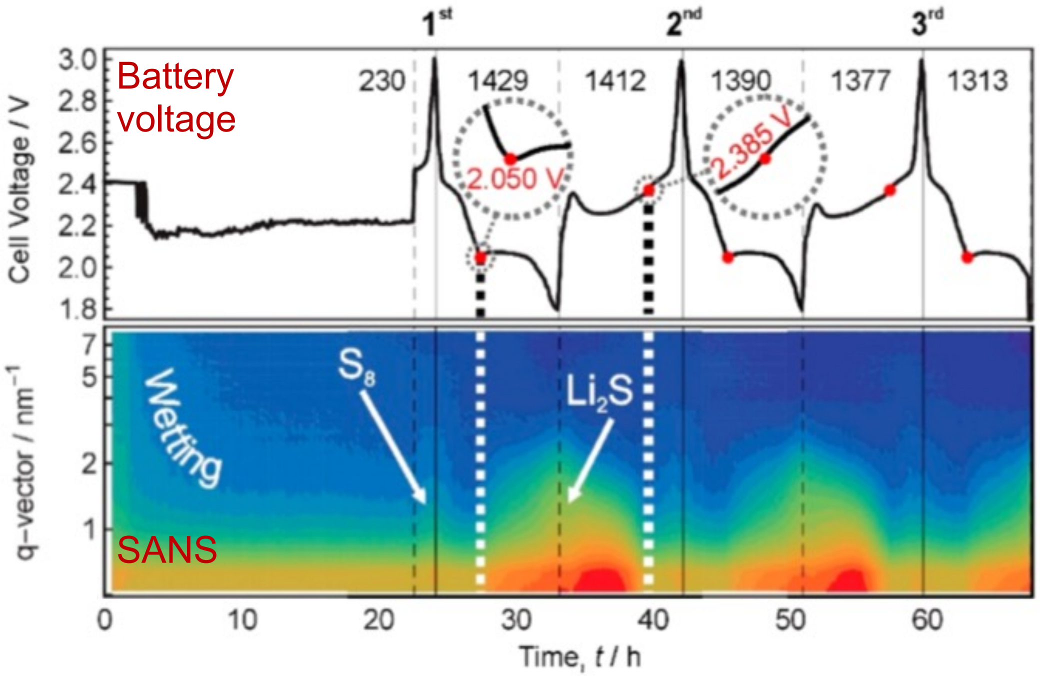

ACS NANO
Cite This: ACS Nano 2019, 13, 10233−10241
www.acsnano.org

Operando Analysis of a Lithium/Sulfur Battery by Small-Angle Neutron Scattering

Sebastian Risse,*,† Eneli Härk,† Ben Kent,† and Matthias Ballauff†,‡
†Institute for Soft Matter and Functional Materials, Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn Meitner Platz 1, 14109 Berlin, Germany
‡Institute of Physics, Humboldt-University Berlin, Unter den Linden 6, 10099 Berlin, Germany

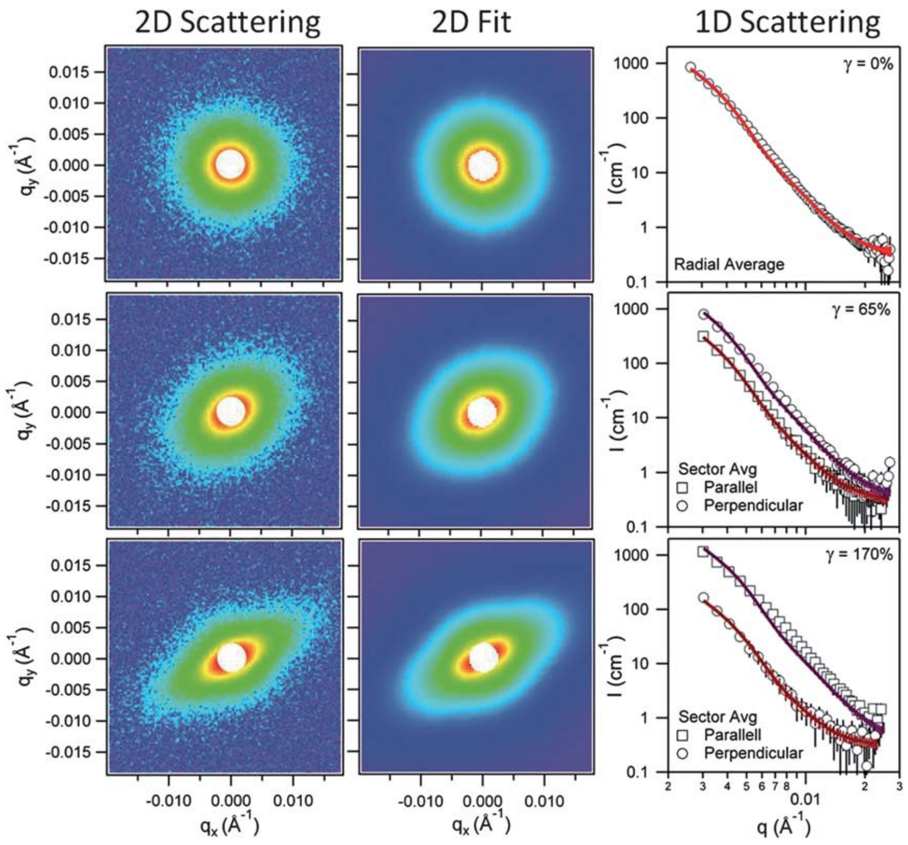
Supporting Information

Ref: **ACS Nano 13, 10233 (2019)**

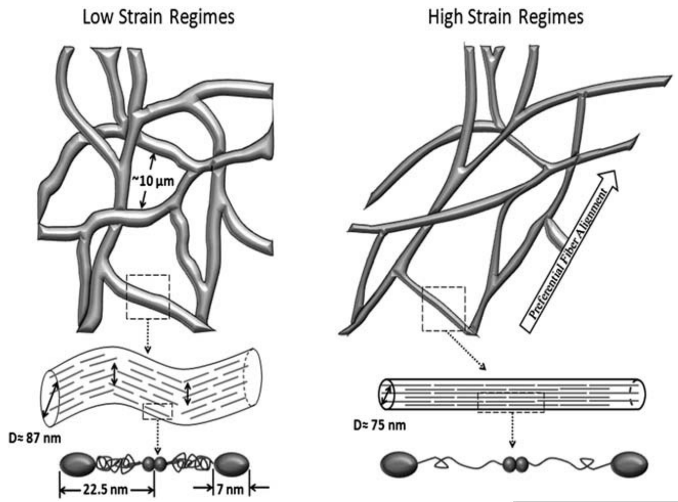


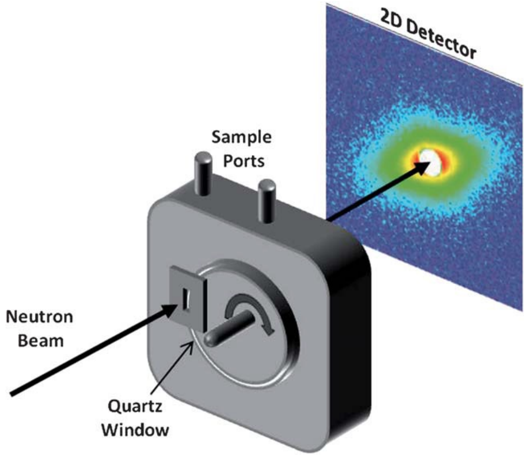
SANS for Soft Matter, Materials & Bioscience

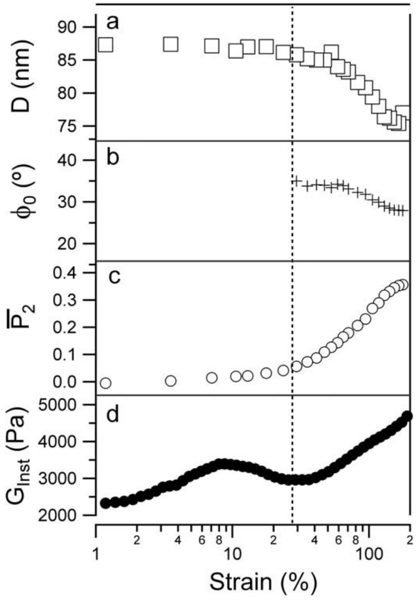
Fluid flow, e.g. rheology



Weigandt, Porcar and Pozzo, *Soft Matter*, 2011, **7**, 9992

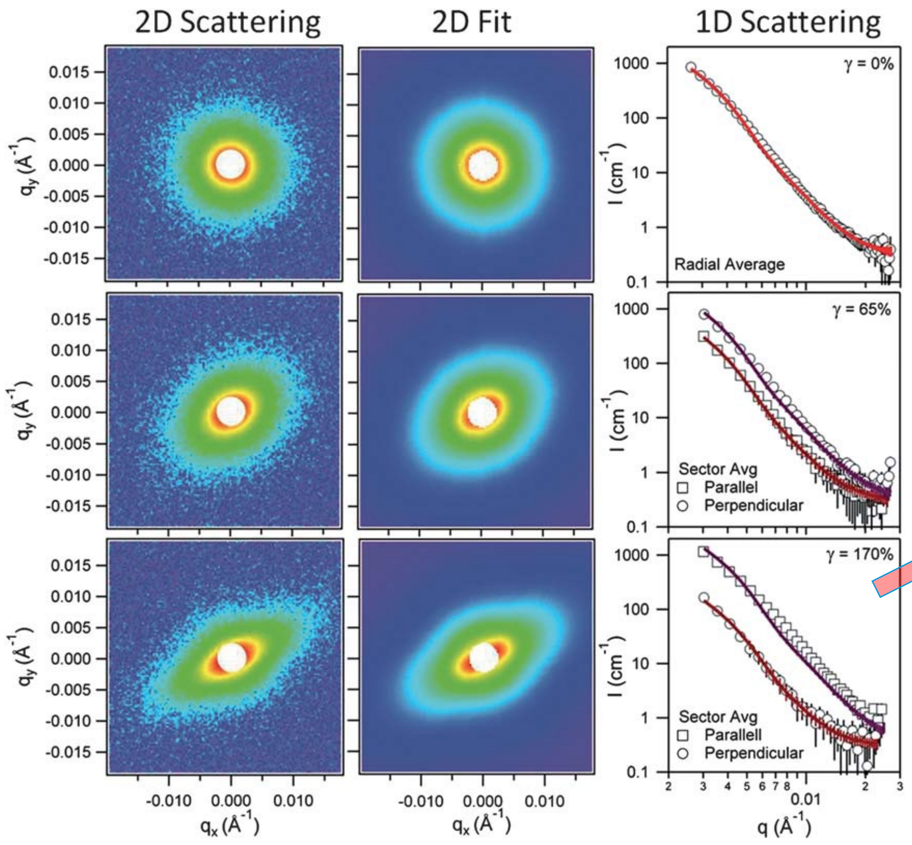




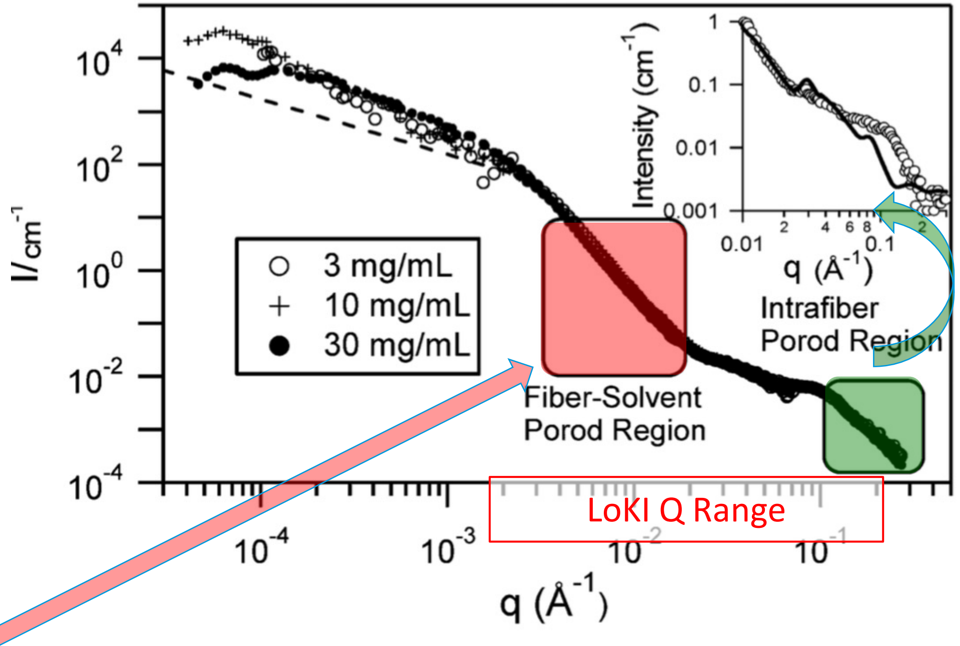


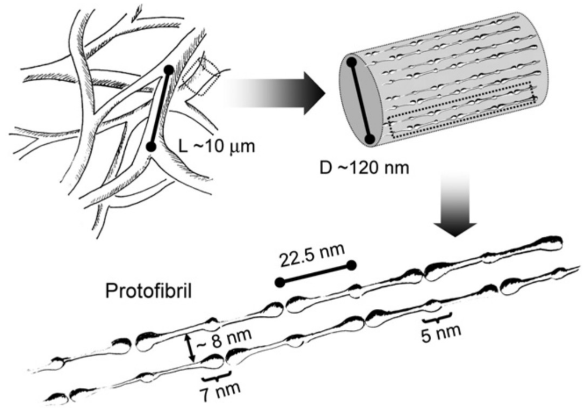
SANS for Soft Matter, Materials & Bioscience

Fluid flow, e.g. rheology



Weigandt, Porcar and Pozzo, *Soft Matter*, 2011, **7**, 9992



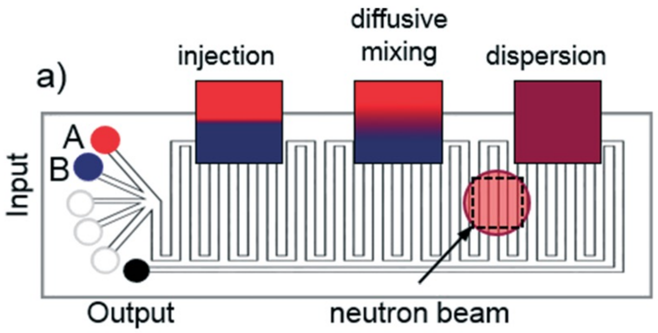


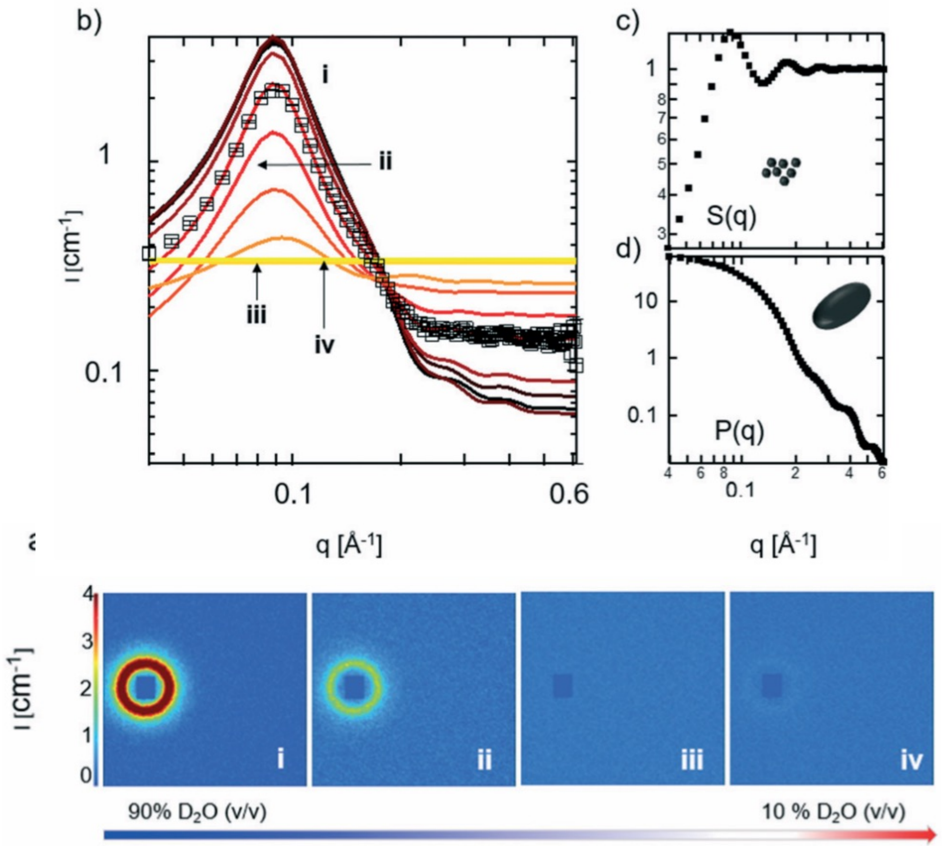
@LoKI: wider simultaneous Q-range.
Probe structural effects of shear over wider size range

SANS for Soft Matter, Materials & Bioscience

Microfluidics

High-throughput mixing & tailored flow geometry





@LoKI: small sample apertures, high throughput, large parameter space

Adamo *et al.*, *Lab Chip*, 2017, **17**, 1559

SANS for Soft Matter, Materials & Bioscience

Weakly scattering biological samples

PLOS | BIOLOGY

RESEARCH ARTICLE

The in vivo structure of biological membranes and evidence for lipid domains

Jonathan D. Nickels[1,2,3☯], Sneha Chatterjee[2,4☯], Christopher B. Stanley[2], Shuo Qian[2], Xiaolin Cheng[5,6], Dean A. A. Myles[2], Robert F. Standaert[1,2,4,6*], James G. Elkins[4,7*], John Katsaras[1,2,3*]

1 Shull Wollan Center—A Joint Institute for Neutron Sciences, Oak Ridge National Laboratory, Oak Ridge, Tennessee, United States of America, **2** Biology and Soft Matter Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee, United States of America, **3** Department of Physics and Astronomy, University of Tennessee, Knoxville, Tennessee, United States of America, **4** Biosciences Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee, United States of America, **5** Center for Molecular Biophysics, Oak Ridge National Laboratory, Oak Ridge, Tennessee, United States of America, **6** Department of Biochemistry & Cellular and Molecular Biology, University of Tennessee, Knoxville, Tennessee, United States of America, **7** Department of Microbiology, University of Tennessee, Knoxville, Tennessee, United States of America

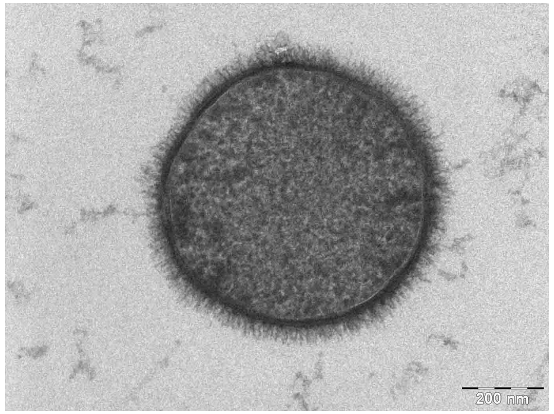
☯ These authors contributed equally to this work.
* standaertrf@ornl.gov (RFS); elkinsjg@ornl.gov (JGE); katsarasj@ornl.gov (JK)

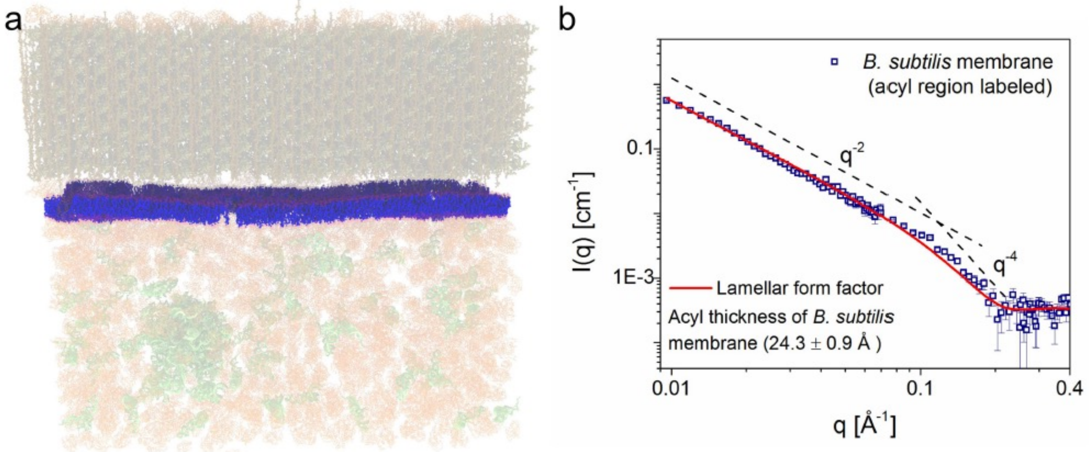
Check for updates

e.g. SANS from perdeuterated living cells with hydrogen labelled cell membrane

→ 4h on BioSANS (ORNL) @ 5mg/ml cells

@LoKI: shorter counting times / higher throughput and low background





Probing viral infection pathways using time-averaged and energy-resolved neutron scattering techniques

J|A|C|S
JOURNAL OF THE AMERICAN CHEMICAL SOCIETY
pubs.acs.org/JACS
Article

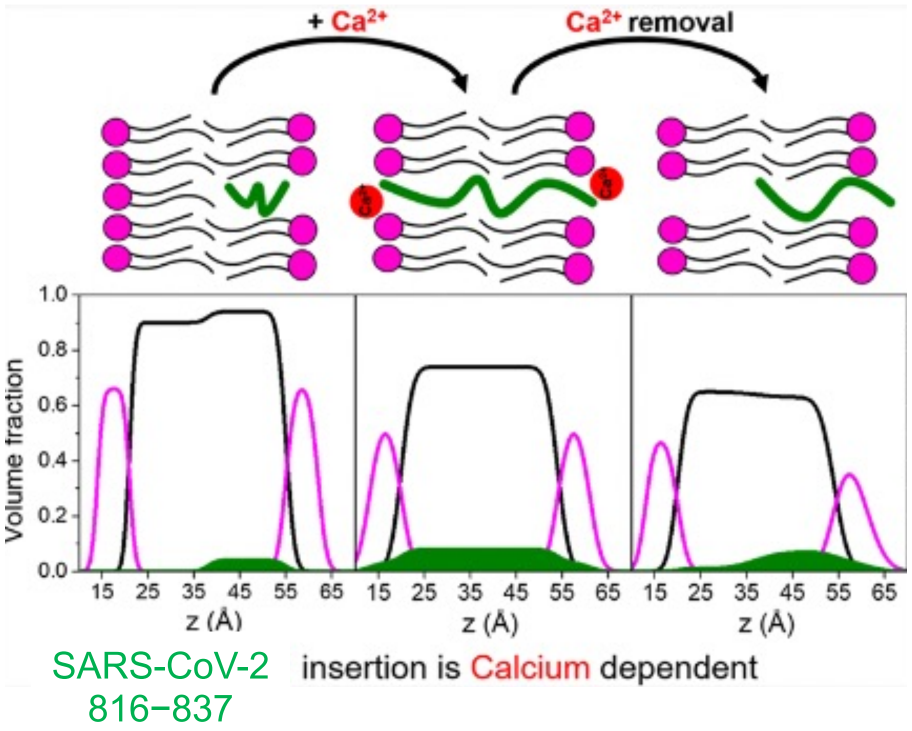
Strikingly Different Roles of SARS-CoV-2 Fusion Peptides Uncovered by Neutron Scattering

Andreas Santamaria, Krishna C. Batchu, Olga Matsarskaia, Sylvain F. Prévost, Daniela Russo, Francesca Natali, Tilo Seydel, Ingo Hoffmann, Valérie Laux, Michael Haertlein, Tamim A. Darwish, Robert A. Russell, Giacomo Corucci, Giovanna Fragneto, Armando Maestro,* and Nathan R. Zaccai*

Cite This: *J. Am. Chem. Soc.* 2022, 144, 2968–2979
Read Online

Ref: **J. Am. Chem. Soc., 144, 2968 (2022)**

Structural information from **specular neutron reflectometry** and **small-angle neutron scattering**, complemented by dynamics information from **quasi-elastic and spin–echo neutron spectroscopy**, revealed strikingly different functions encoded in the different SARS-CoV-2 Spike fusion peptides, as well as the influence of calcium and cholesterol, in the fusion process between viral and host membrane.



3

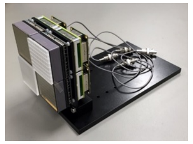
SANS at the ESS

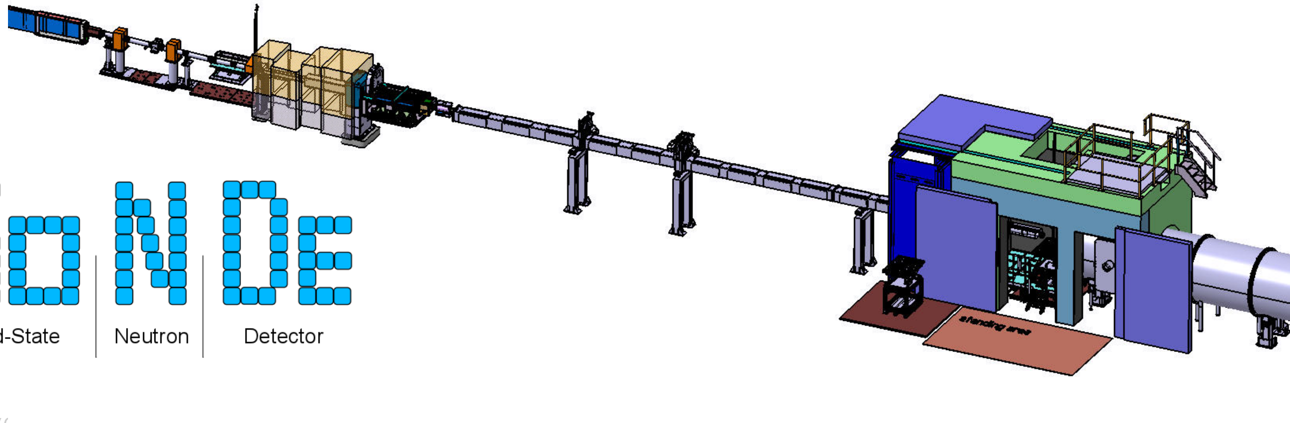
SKADI High Resolution SANS

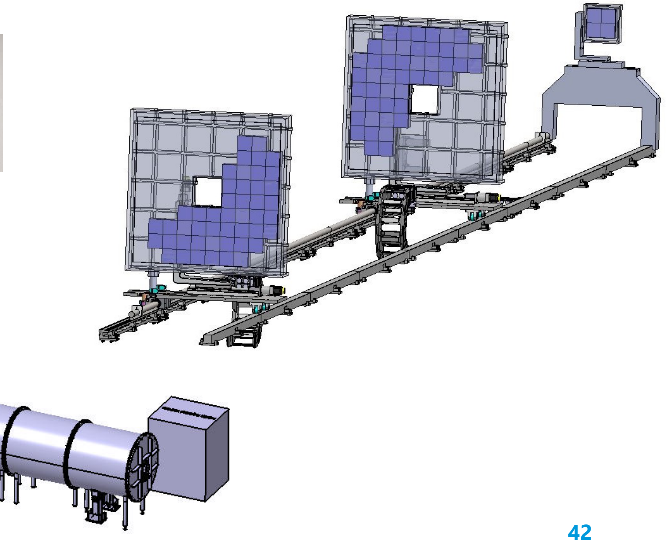
S. Jaksch, H. Frielinghaus (JCNS), J. Jestin (LLB), R. Hanslik (FJZ), S. Desért (LLB)

- High-flux neutron extraction by optimized deflector
- Separate long/short wavelength polarization with supermirrors
- 4, 8, 14 and 20 m collimation settings
- VSANS: Down to ~10^{-5}Å^{-1}
- SoNDe : Dedicated detector development for best use of high-flux and single shot measurements, achieving large Q-coverage.

Quick Facts	
Moderator	Cold (max @ ~3 Å)
Length	58 m
Q-Range	10^{-4} – 1 Å^{-1}
Flux at sample position	7.7×10^{8} n s^{-1} cm^{-2}
Standard Mode (14 Hz)	
Wavelength Band	5 Å
Wavelength Range	3 – 21 Å
Momentum Resolution	ΔQ/Q= 2-7 %

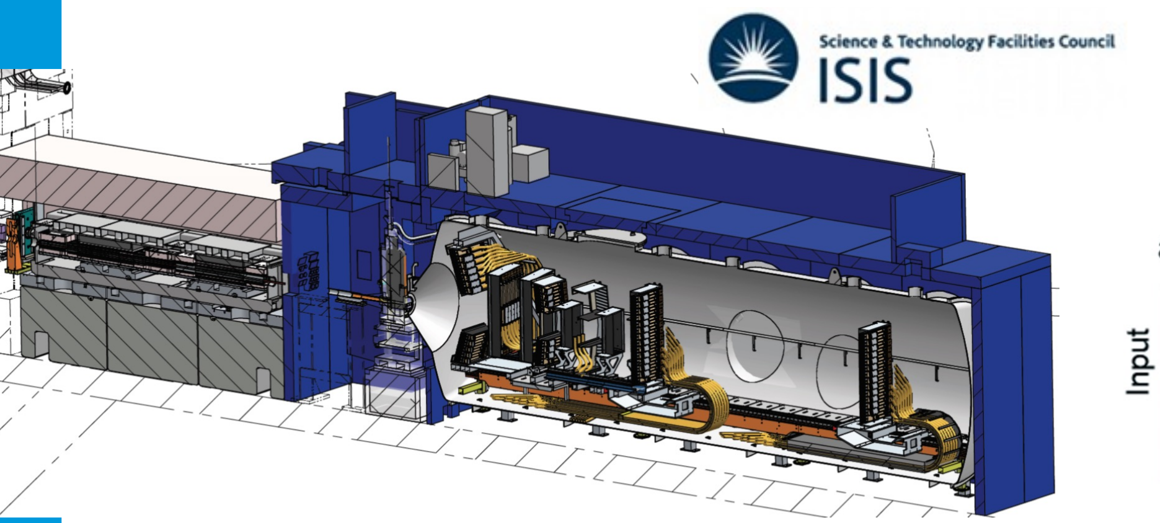






SoNDe
Solid-State | Neutron | Detector

LOKI Broad Band SANS

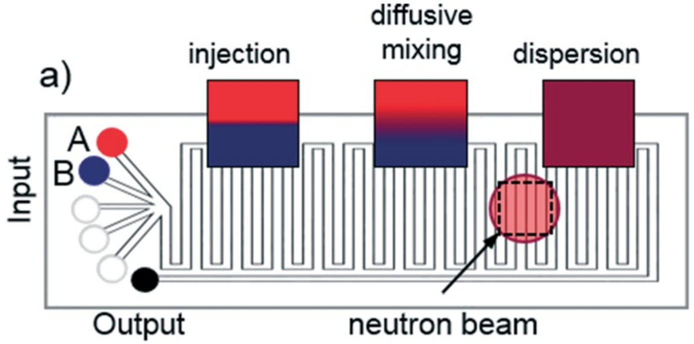


→ high flux, wide simultaneous size range, and a flexible sample area.

ABILITIES:

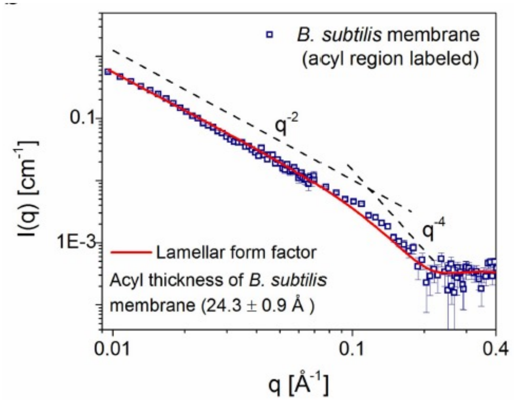
- Investigate **multiple length scale** systems (simultaneously 0.5-300 nm)
- Perform **"single-shot" kinetic measurements** on sub-second timescales.
- Perform experiments that use flow e.g. rheology & microfluidics **with small beam sizes**
- **High throughput** of regular SANS measurements

Microfluidic SANS:
High Throughput Mixing & Tailored Flow Geometry



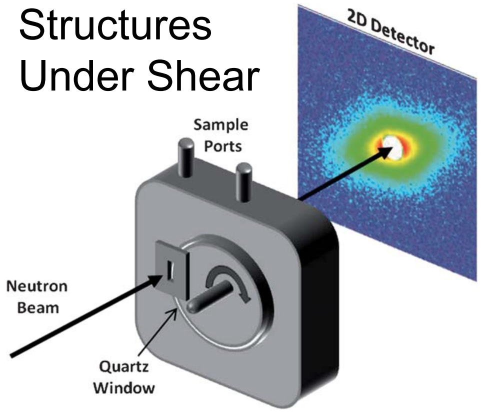
Lab Chip, 2017, **17**, 1559

Biological Samples:
Weak Scatterers & Dilute Solutions



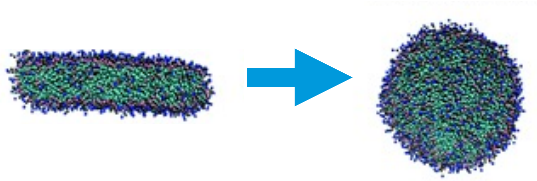
PLoS Bio, 2017, **15**, e2002214

Rheo-SANS:
Structures Under Shear



Soft Matter, 2011, **7**, 9992

Non-Equilibrium Studies:
Self-Assembly & Kinetics



Colloid Polym Sci, 2010, **288**, 827

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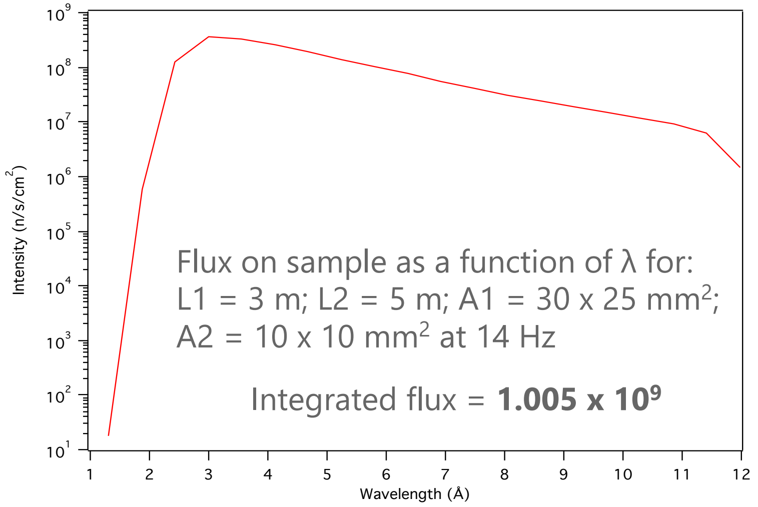
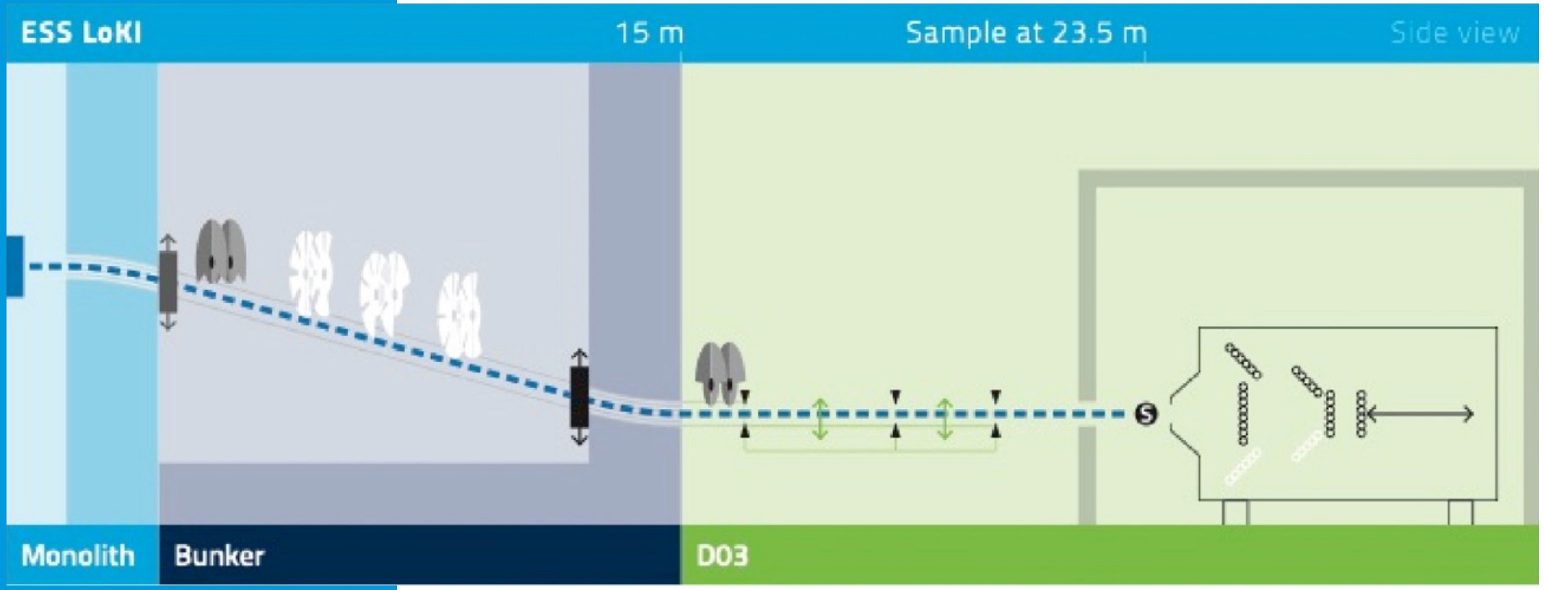
LoKI: SANS for Soft Matter, Materials & Bioscience





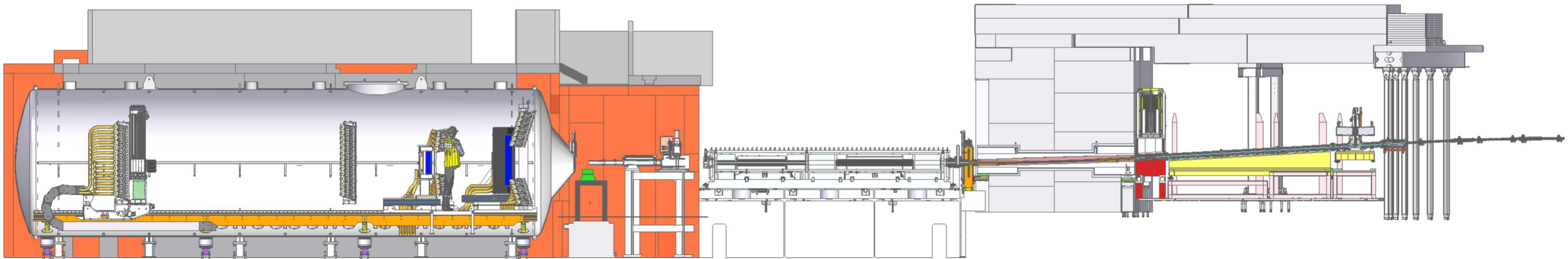
LoKI Timeline

Due to be finished construction in mid-late 2023

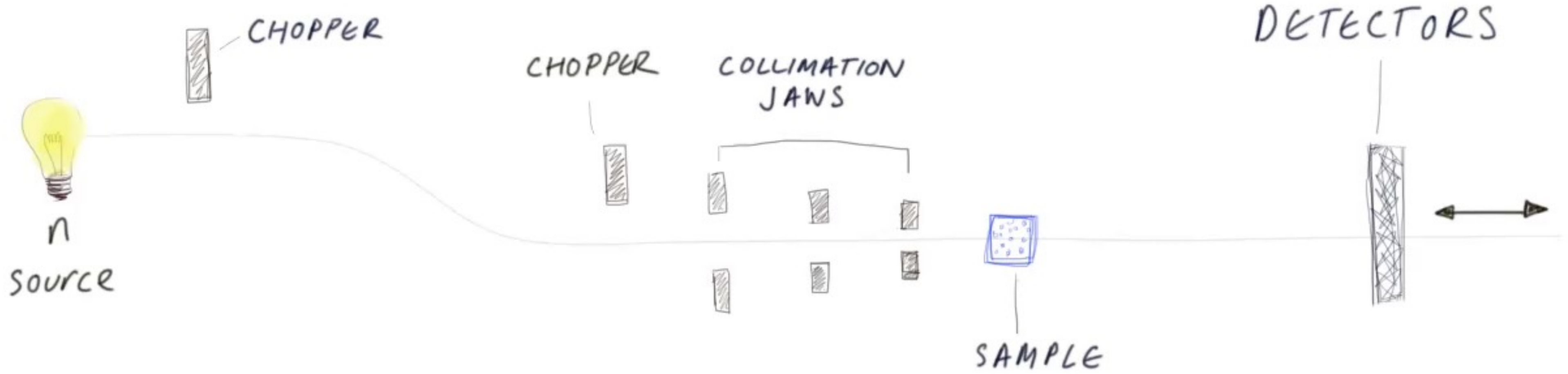
We're here

Instrument selected! → Preliminary engineering design → Final engineering design → Pre-build at ISIS → Construction & installation in Lund → Beam test & commissioning → Operations & continuous development

Early science



The Design



Requirements

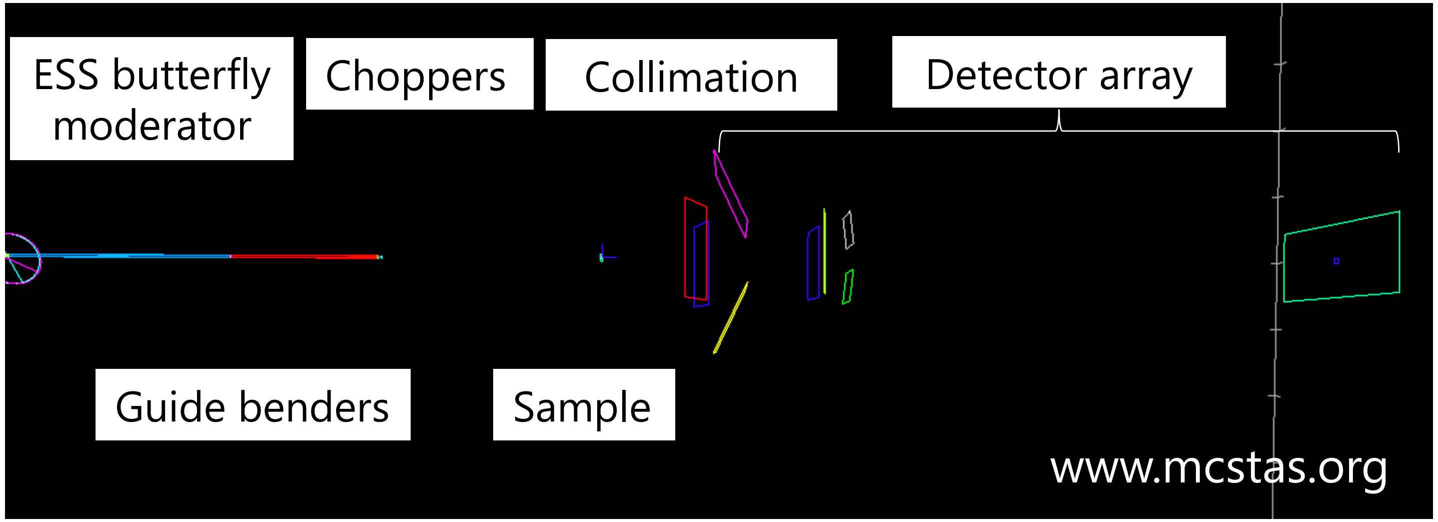
1. Super bright **source** & cold moderator ✓
2. **Guide** to tunnel the neutrons down to our sample position
3. **Choppers** to shape and define our neutron profile
4. **Collimation** jaws (pinholes) to “shape” our beam
5. **Environments** to support our samples
6. Efficient **detectors** with good resolution and wide coverage to measure our scatter

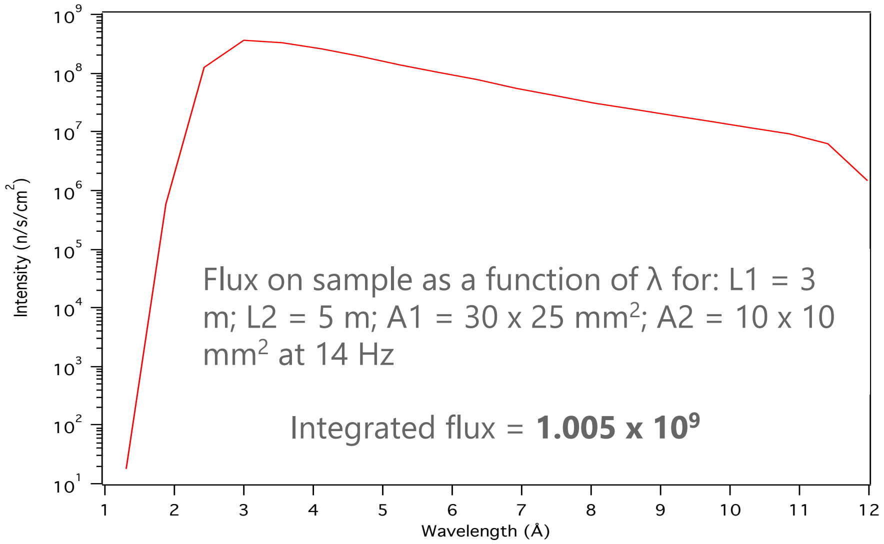
Other considerations

1. Vacuum
2. Shielding (in **and** out)
3. Speedy electronics and state-of-the-art software

Proposing & optimising a design

Optimisation of the instrument design is done using McStas neutron transport code





Defining our beam : Choppers

Periodically interrupt the beam for a well-defined period of time

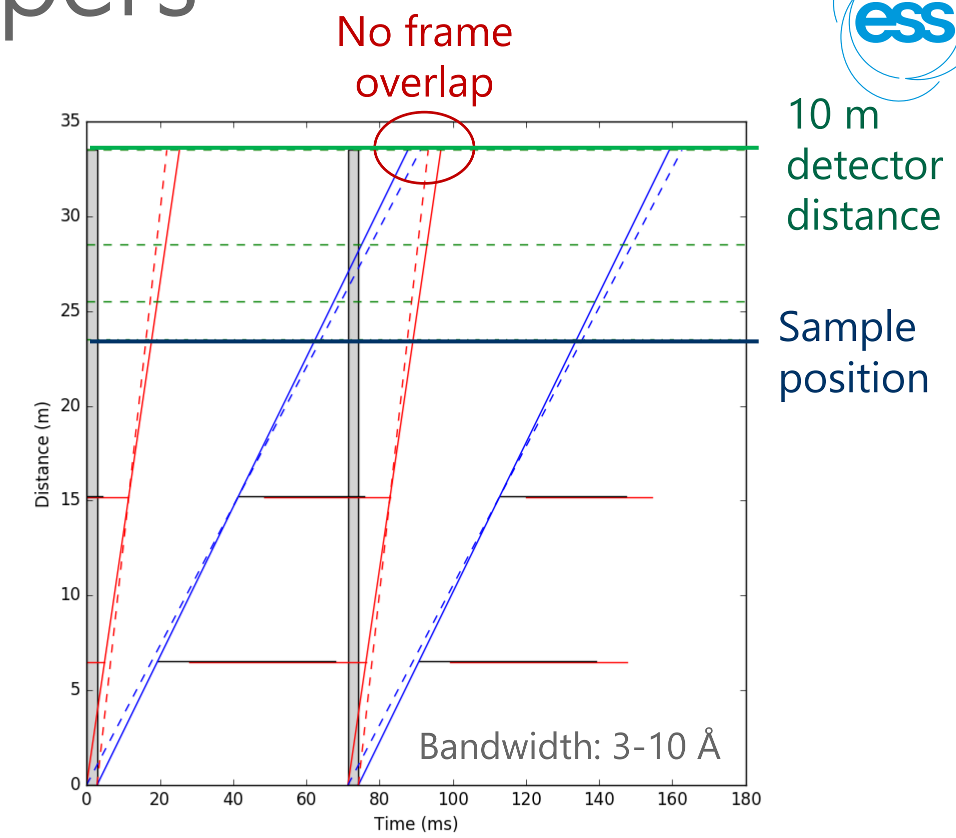
Requirements

- Cut the bandwidth down from 0.4 Å and 20 Å to a defined wavelength band of up to 10 Å at 14 Hz and up to 20 Å at 7 Hz
- Prevent overlap between sequential pulses
- Operate in monochromatic mode

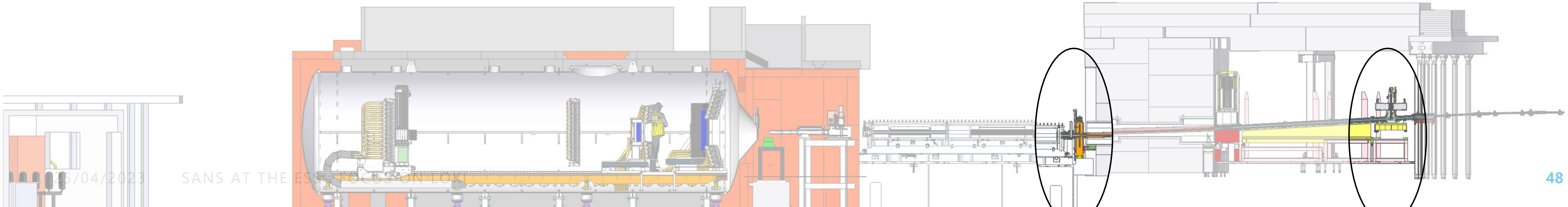
To do this, we define:

- Disk openings
- Rotation speed
- Position along the beam

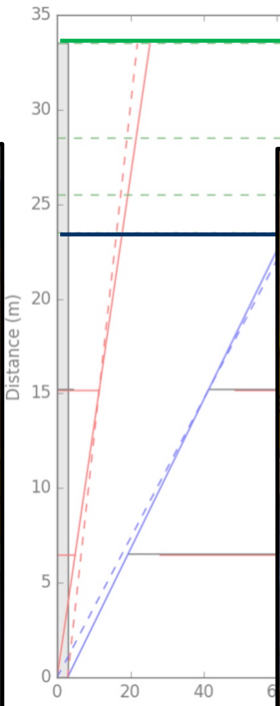
*Option for resolution enhancing choppers



e.g. Time-distance diagram for 14 Hz operation with rear detector at 10 m from sample



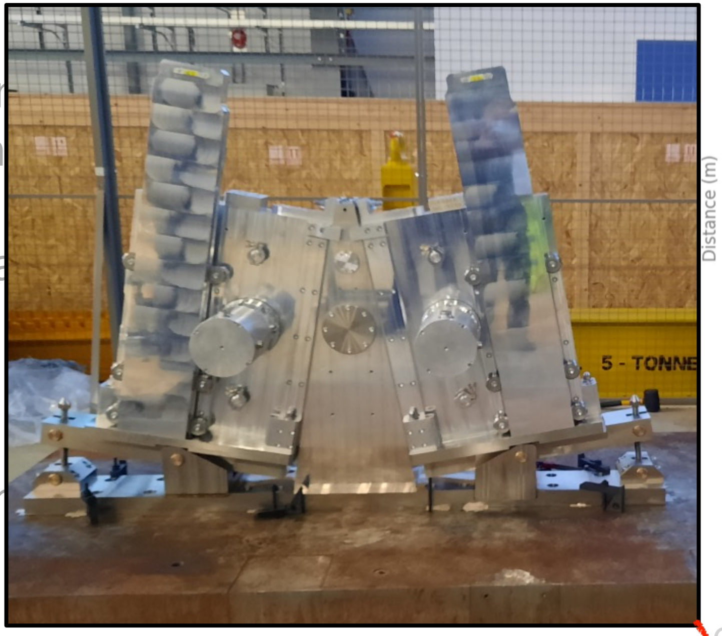
Defining our beam : Choppers

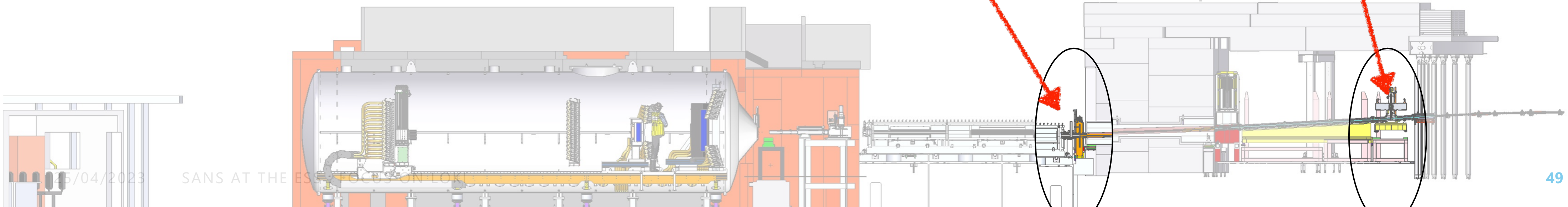


e.g. Time-distance diagram for 14 Hz operation with rear detector at 10 m from sample

Requirements
- Cut the bandwidth dowr to a defined wavelength 14 Hz and up to 20 Å at
- Operate in monochroma

*Option for resolution enhar



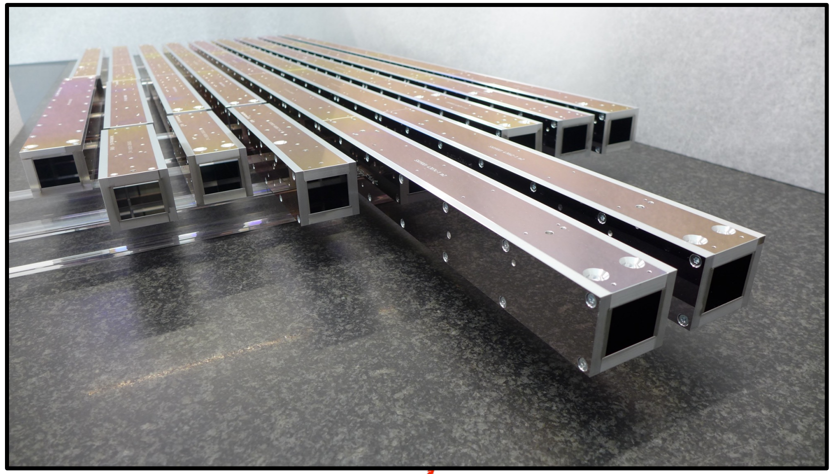


Defining our beam : **neutron guide**

Transporting the good neutrons, removing the "bad" ones

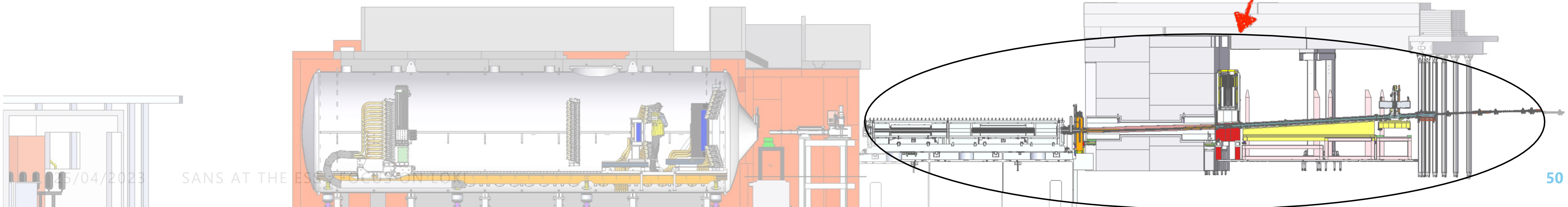
Requirement:

- **Transport neutrons** from the moderator to the sample with 100% brilliance transfer within the selected wavelength and divergence range
- **Prevent the transport** of high energy neutrons
- **Signal-to-noise** to be the best it possibly can possibly be



What we can do:

- Use straight highly reflective guide (m=2) under vacuum
- Two multichannel benders (m=3) = **twice** out of line-of-sight
- Smaller beam size (25 mm × 30 mm (V × H)) to minimise transport of background



Defining our beam : **Collimation**

Controlling the size and divergence of the beam (similar to reactor SANS)

Generally, the biggest challenge in the design of any SAS instrument is to separate the direct beam from the scattered radiation at small angles (<0.1°).

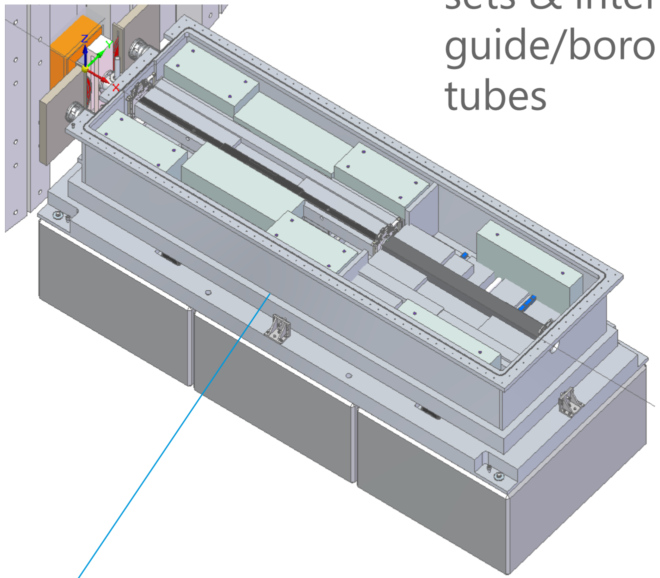
Requirements

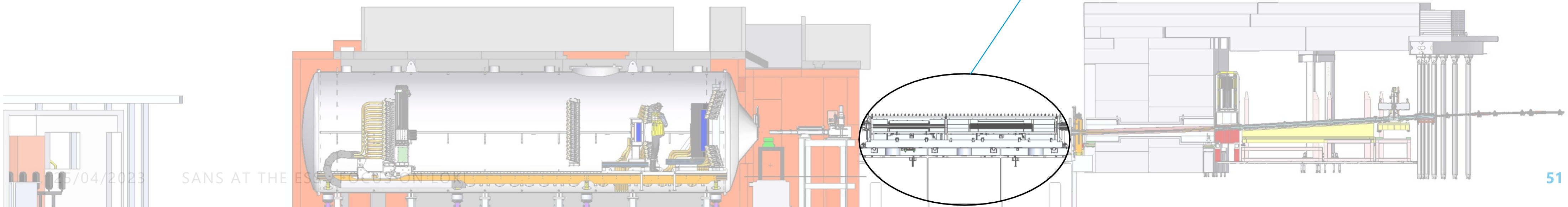
- Control the **size** and **divergence** of the beam

To do this:

- 4-jaw slit sets at 8, 5 & 3 m before the sample position
- Variable-sized apertures at the sample position
- Platform to switch between evacuated boron-lined tubes (collimation) or sections of m=2 guide

Collimation vacuum tank containing slit sets & interchanged guide/boron-lined tubes

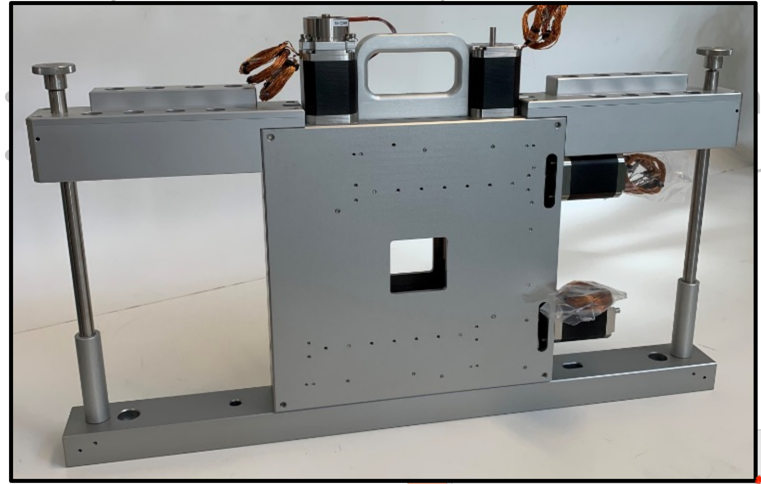




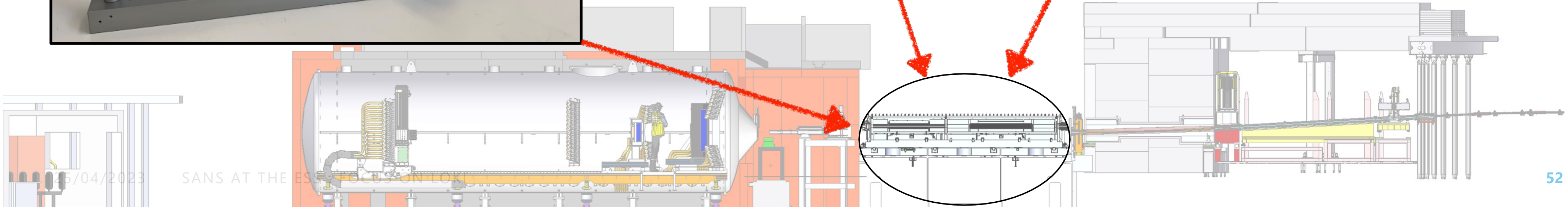
Defining our bear … on

Requirements
- Control the **size** and **divergence** of

What we have:
- 4-jaw slit sets at 8, 5 & 3 m before t



…mple position
…uated boron-lined
…m=2 guide



Shielding

Crucial for personal protection as well as background reduction

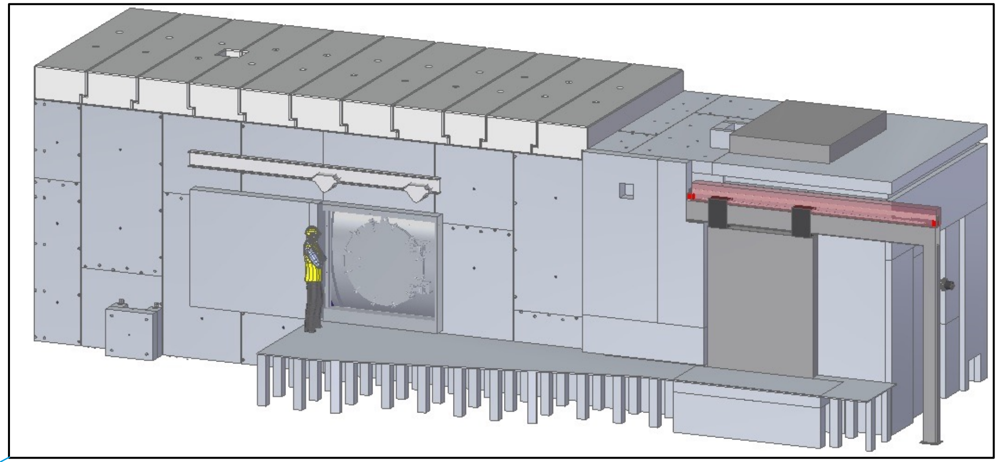
Requirements

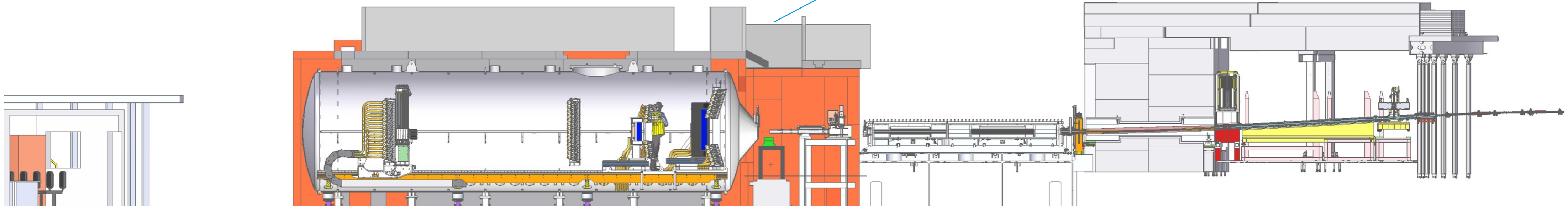
- **Protect** users, staff, the public from radiation (highest priority)*
- **Improve background**: Best signal-to-noise possible

To do this, we:

- Run simulations to identify the amount of radiation present, where are the hotspots?
- Steel and concrete caves around the entire instrument

*in addition to the other personal protection systems in place!



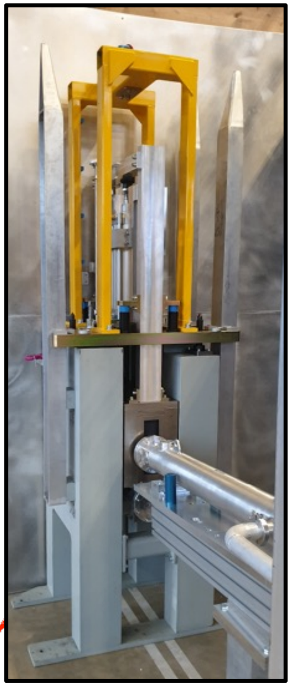


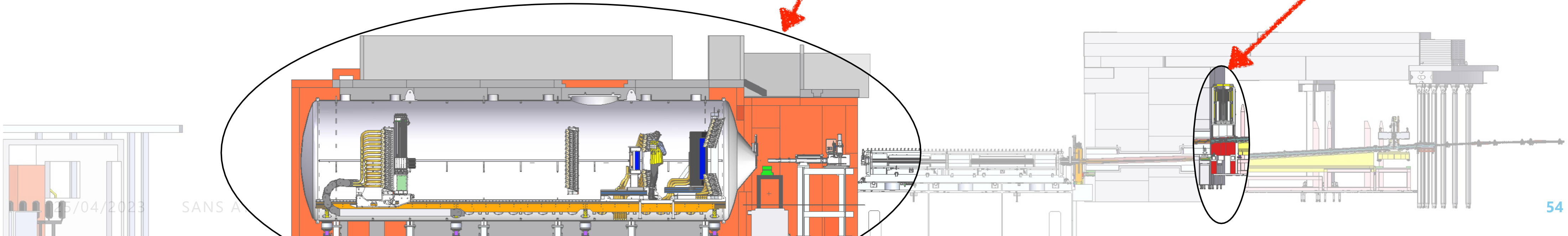
Shielding

Crucial for personal protection as well as background reduction

Requirements
- Fulfill radiation requirements
- **Improve background**: Best signal-to-noise p

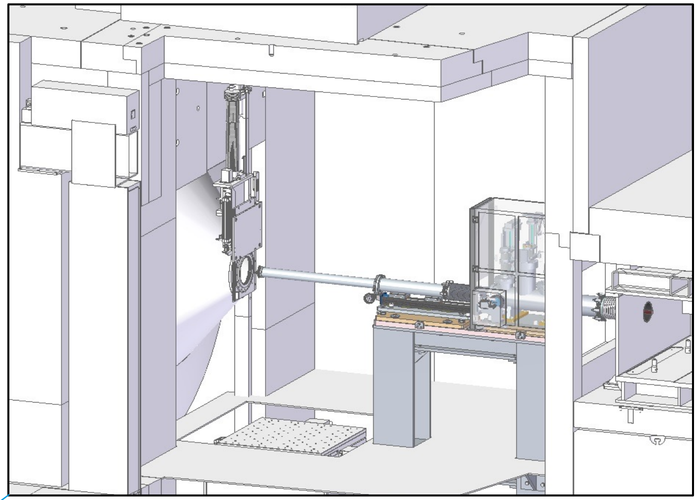
To do this, we:
- Steel and concrete caves around the entire instrument
- Heavy shutter to allow access to the sample area to change samples

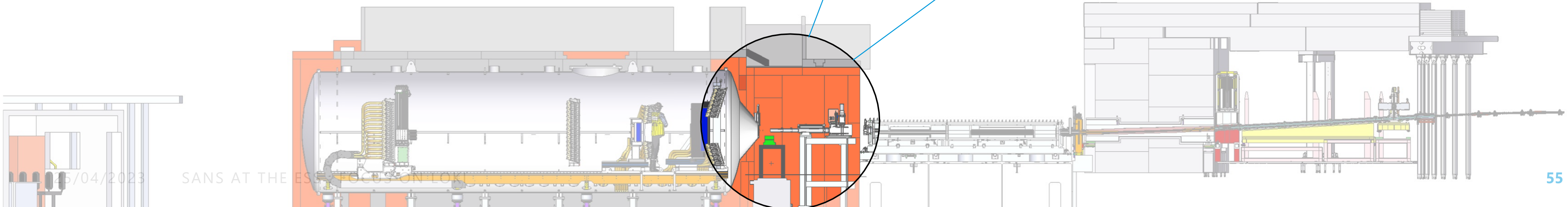




Sample environment

How best can we support our science case and take advantage of the wide simultaneous q-range and high flux?





Sample environment

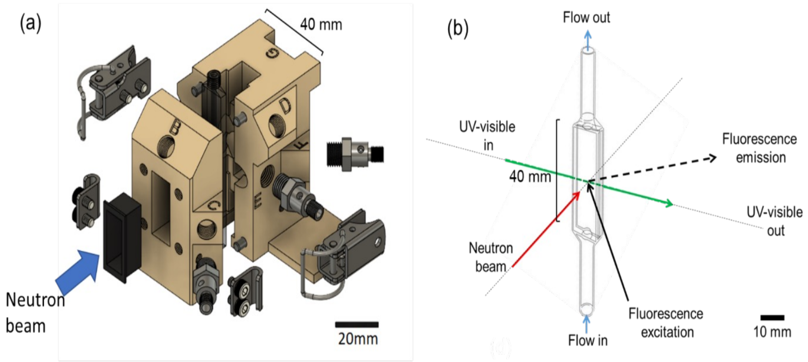
The "off-the-shelf" variety

- **Thermostated cell holder**
- **Rheometer**
- **Flow cell with HPLC pumps**
- **Rotating cell holder**
- **Couette shear** (higher shear rates)
- Plate-plate shear (for e.g. polymers)
- 2.5T electromagnet
- Humidity chamber
- **Stopped-flow equipment**
- Stress/strain rig (load capacity for stretching polymers)
- Cryostats

Custom-built sample environments

e.g. **NuRF** (Swedish VR collaboration)

In situ fluorescence, UV/vis absorption spectroscopies, densiometry on a continuous flow cell

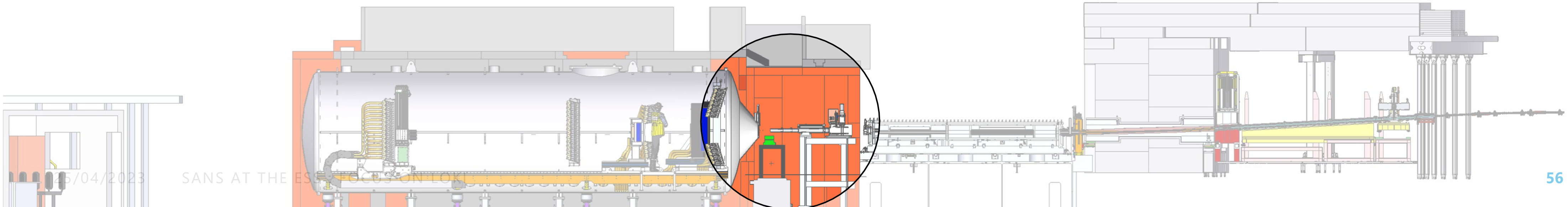


Available on Larmor (ISIS, UK)

e.g. **Flexiprob** (German collaboration)

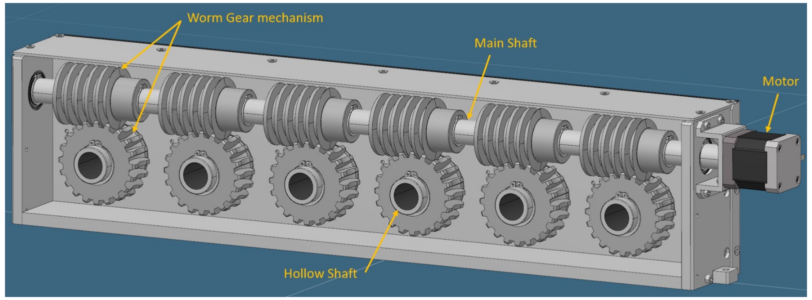
Easily switchable set-up between:
- in situ dynamic light scattering
- Foam cell
- Humidity chamber for GiSANS (shown)

Prototyped on KWS-1 (JCNS, Germany)

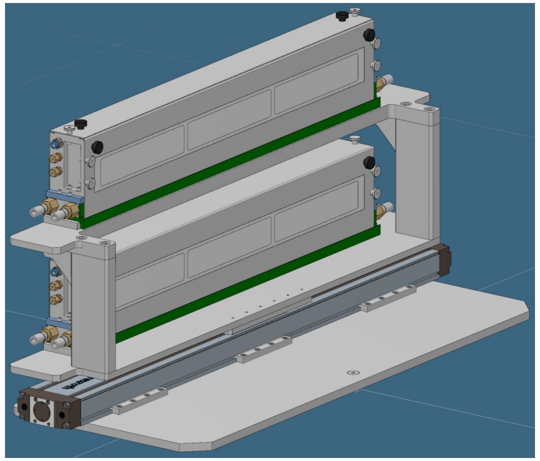


Sample Environment

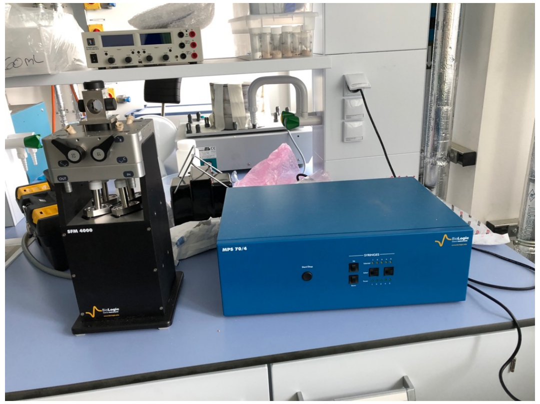
Rotating cell holder



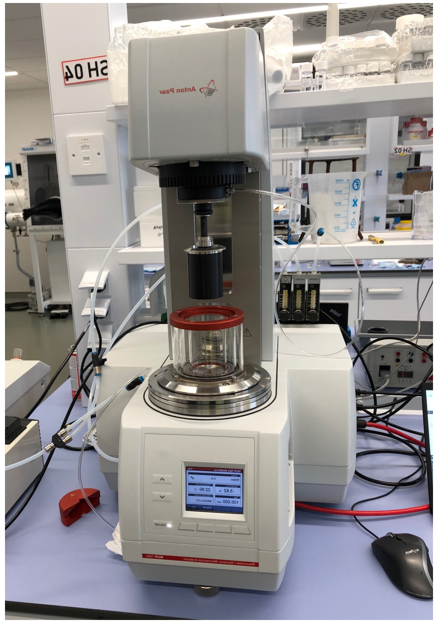
SANS changer

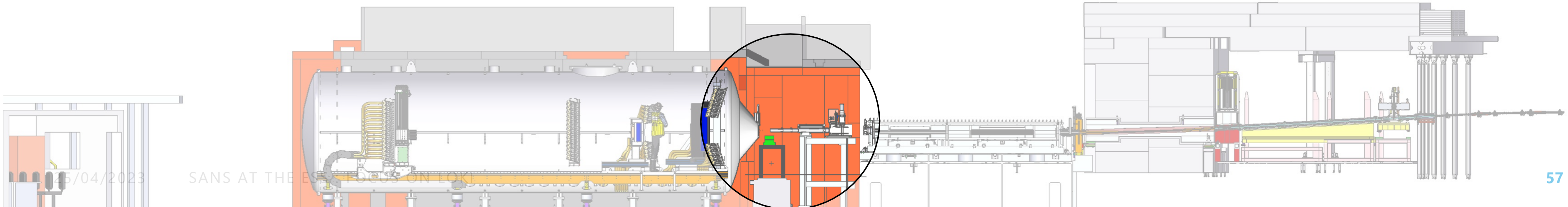


stop flow cell set-up



Rheometer



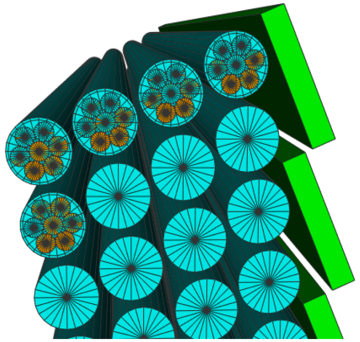


Detector System

Novel ^{10}B-based straw tubes design typically used in security

Efficiency: ~50%-60% at LoKI wavelength
Position resolution: FWHM is ~6 mm up to 350 kHz
Rate capability: 15% rate lost at 2.3 MHz

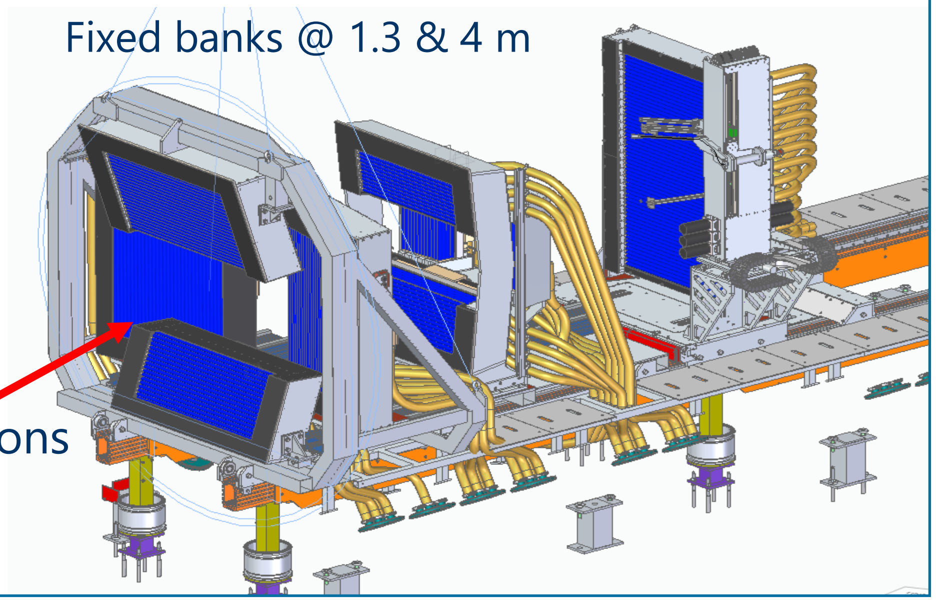
4 layers of Al tubes, each containing 7 boron-coated straws

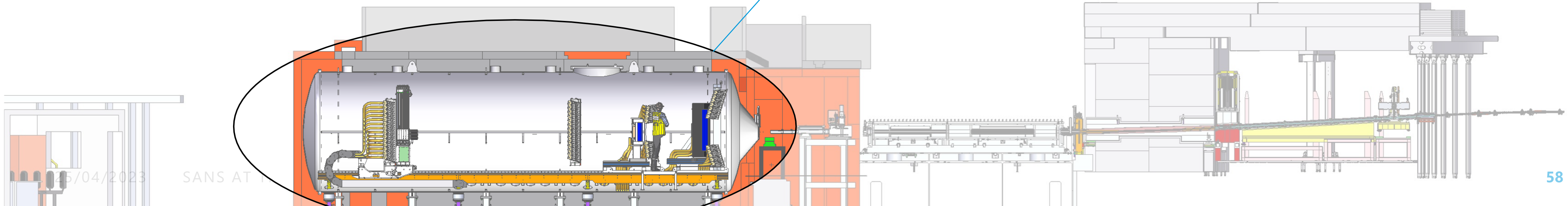


880 tubes x 7 straws x 256 pixels
= **1,576,960 pixels**

Covering 0º to 45º in scattering angle and 360º in azimuthal angle (180º Day 1).

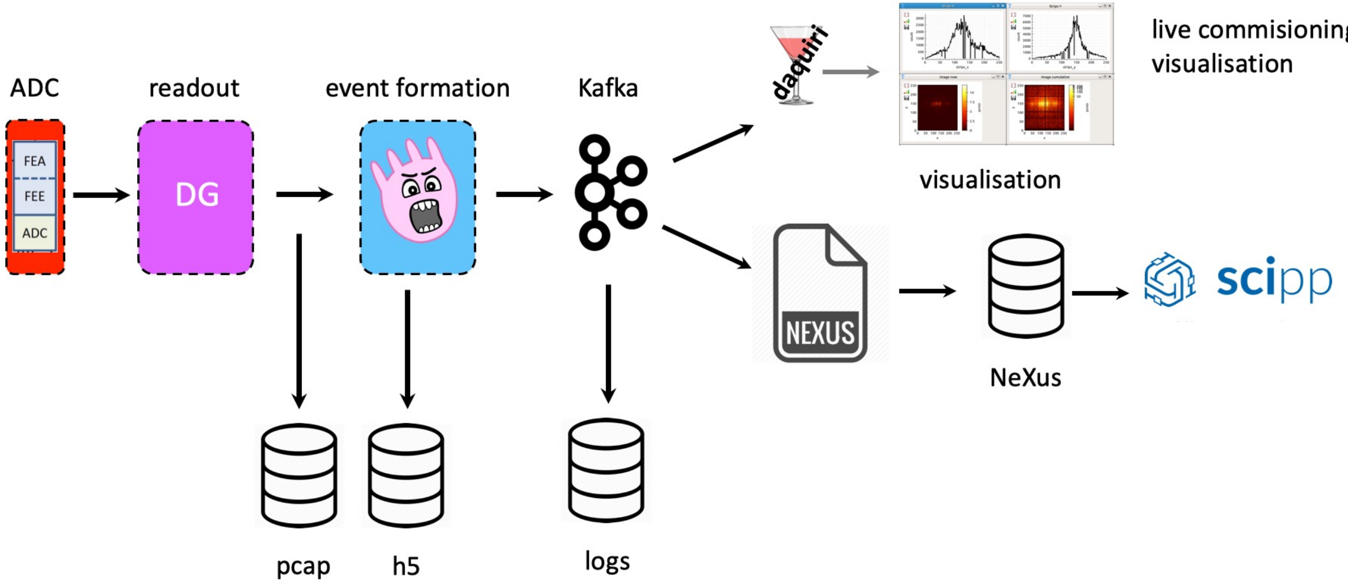
Rear detector moveable between 5 & 10 m

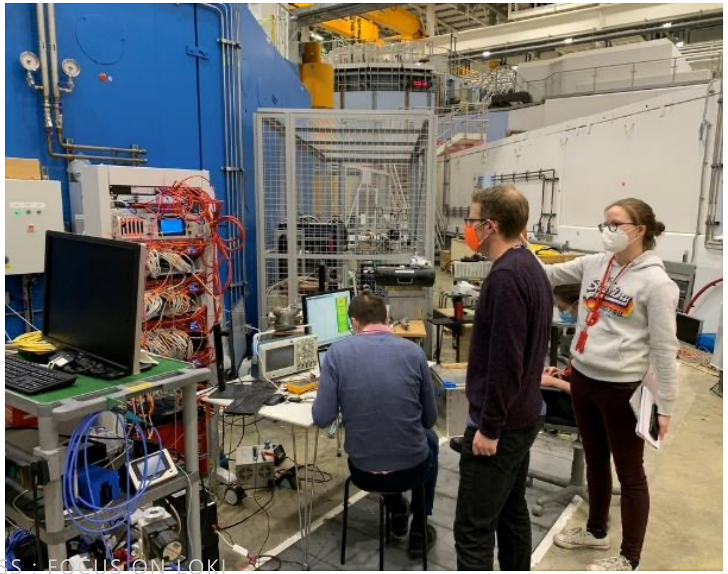


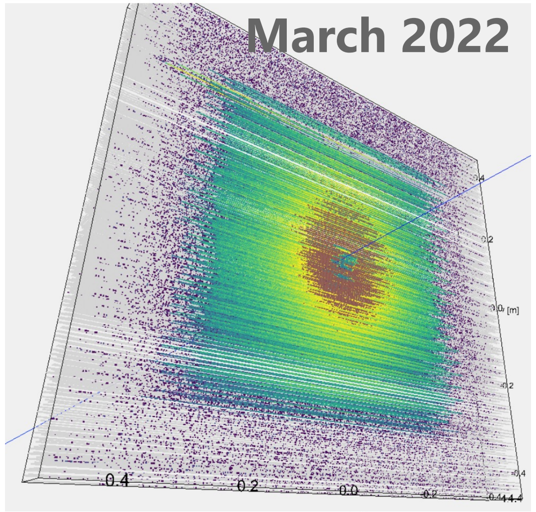


Detector Tests on Larmor (ISIS, UK)

Collected calibration data on the LoKI rear detector using the **full ESS software stack:** Excellent test for Hot Commissioning







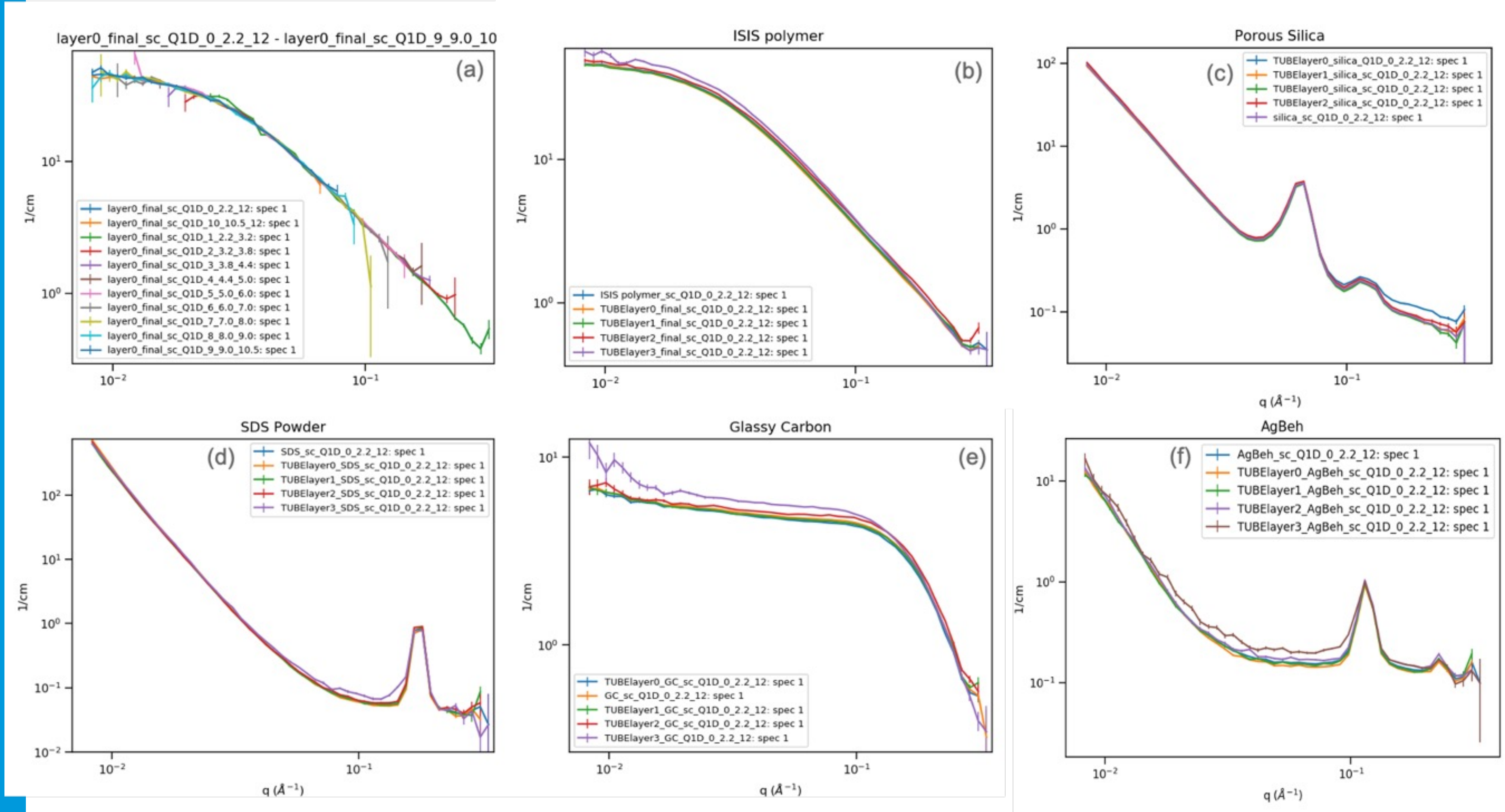
NeXus file displayed in scipp

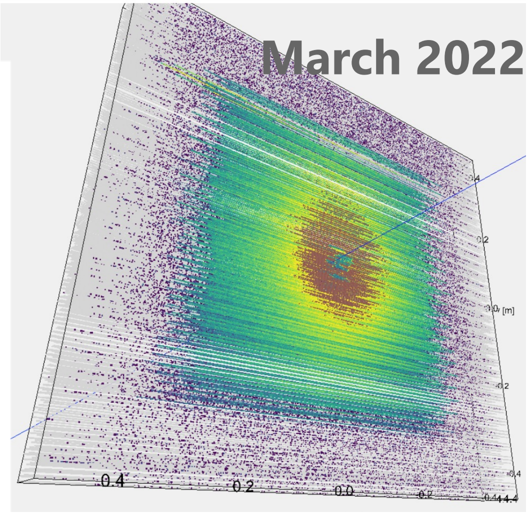
Sample measured:

1. Cd stripped mask
2. Silver behenate
3. SDS powder
4. empty beam
5. blocked beam
6. ISIS standard polymer
7. Silica particles
8. Vanadium

Detector Tests on Larmor (ISIS, UK)

Data reduction in Mantid to be transferred to SCIPP





NeXus file displayed in scipp

Sample measured:

1. Cd stripped mask
2. Silver behenate
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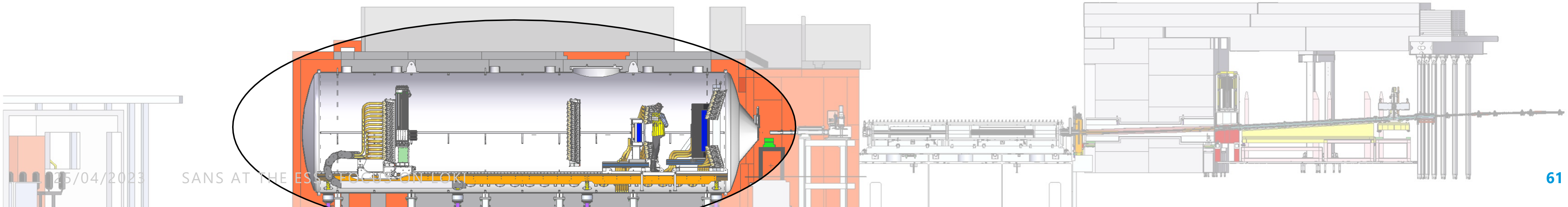
7. Silica particles
8. Vanadium

Detector System

Detector vessel installed at ESS

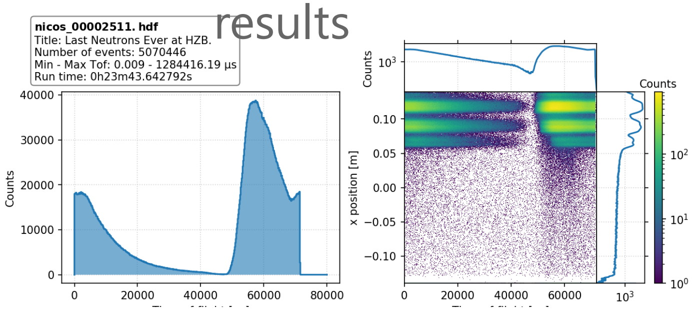
Detector mechanics prebuild at ISIS



Data processing

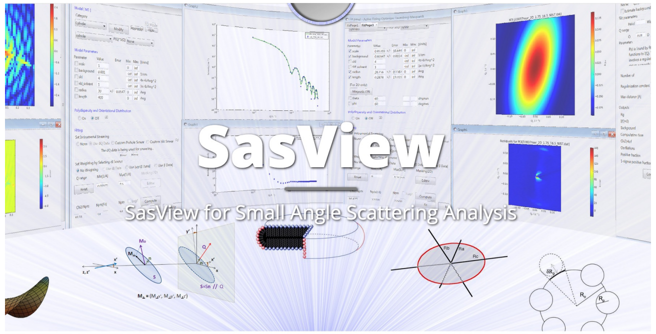
Data catalogue

Scicat is a metadata catalogue allows users to access information about experimental results



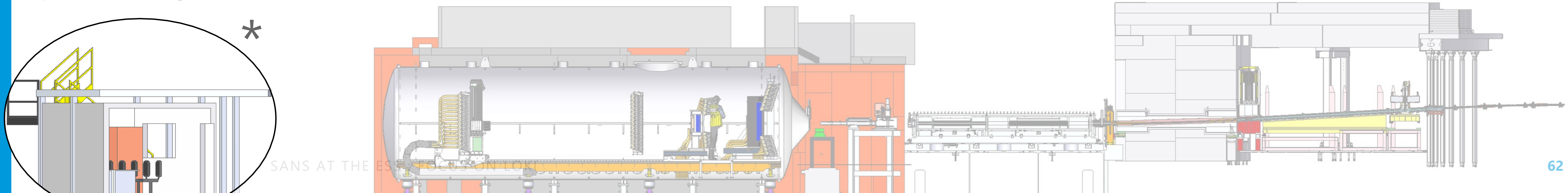
Data visualisation & processing

Data analysis

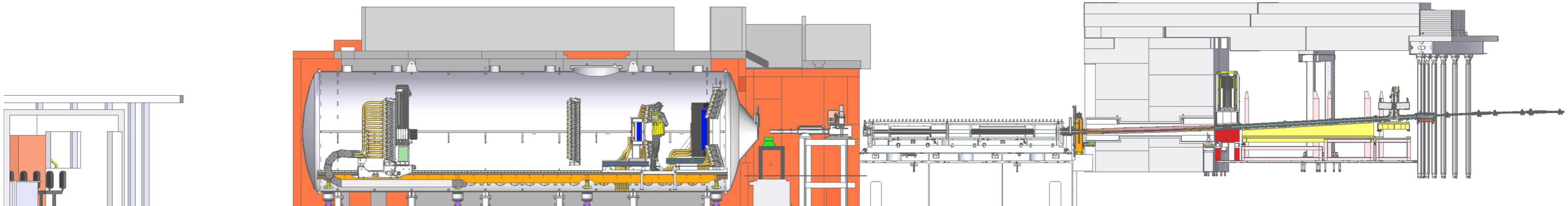


To name a few...

Data storage, & servers for processing in DK (DMSC)



Getting there slowly...



5

Hot commissioning & early science

Once we have LoKI, what will we do with it?

Path from hot commissioning to early science

Stage 1:
Compulsory calibration tests

Standard calibrating samples for SANS:
Vanadium
SDS Powder
Silver Behenate
Latex nanoparticles

Round robin samples:
Glassy carbon (NIST)
Mesoporous silica (FSM-16)

Stage 2:
Early science tests - Samples selected to match the available instrument set-up

INSTRUMENT SET-UP	SCIENTIFIC CAPABILITY	POTENTIAL SAMPLES (using the regular cell holder or pre-commissioned sample environments)
Only the rear detector	Low Q only, length scales of 10-300 nm	Nanogels, surfactant self-assemblies, photoluminescent materials, e.g. conjugated polymers
Wide-angle detector banks	High Q only, length scales of 0.5-50 nm	Crystalline/mesoporous materials, e.g. templated organosilica
Full detector coverage	Simultaneously probe multiple length scales (0.5-300 nm)	Liquid crystal nanoparticles, e.g. hexasomes, cubosomes Wormlike micelles

Stage 3:
Early science - more complex samples/sample environment & full instrument set-up

Work with collaborators and expert users to:

- Investigate multiple length scales
- Perform experiments using flow e.g. rheology & microfluidics
- Use pre-commissioned in situ sample environments

* Samples should be stable for storage & readily available at the instrument
** Samples will be provided by the instrument team or close collaborators

LoKI Early Science

Taking advantage of the wide simultaneous q-range, large sample area & low background

Performance @~0.5 MW:
- Comparable to SANS2D

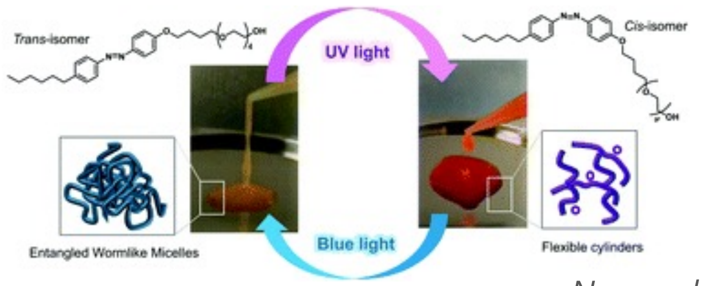
Performance @2 MW:
- ~5x compared to D22 (LoKI@14 Hz)
- ~20x SANS2D (LoKI@7 Hz)

Work with collaborators and expert users to:
- Investigate multiple length scale systems (simultaneously 0.5-300 nm)
- Perform experiments that use flow e.g. rheology & microfluidics
- Carry out work-horse SANS measurements with higher throughput
- Take advantage of pre-commissioned in situ sample environments

Some current ideas…

Photoswitchable worm-like micelles

R. Evans in Cambridge, UK

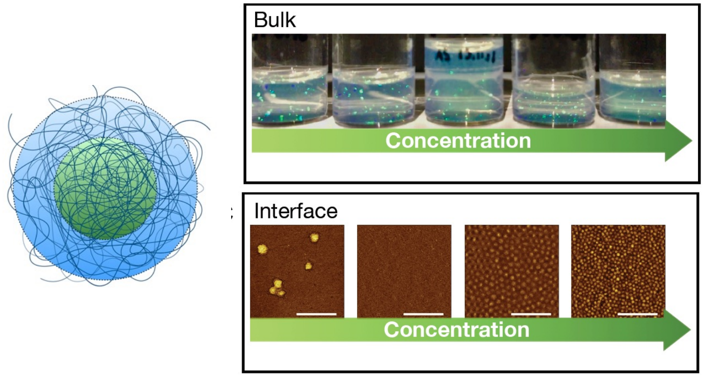


Nanoscale, 2020,**12**, 6300

System under flow ✓
Multiple length-scales ✓
In situ sample irradiation (adaptive sample environment) ✓

Polymeric microgels

A. Scotti in Aachen, Germany

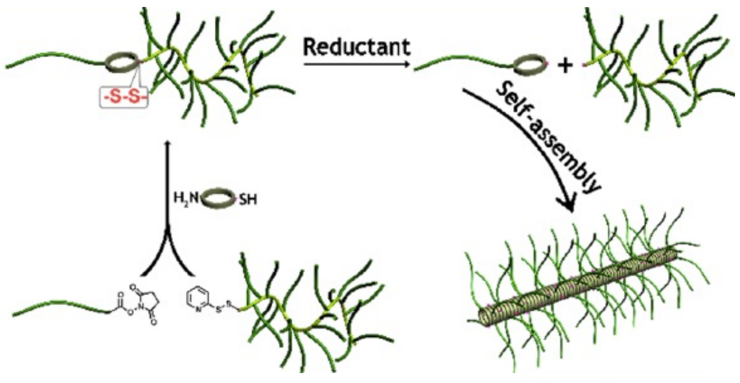


Nature Commun., 2019,**10**, 1418

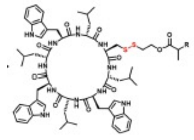
System under flow ✓
Multiple length-scales ✓
Work-horse SANS experiments ✓

Cyclic fluorescent peptides

S. Hall in Warwick, UK



ACS Macro Lett., 2019, **8**, 1347



Multiple length-scales ✓
In situ spectroscopies ✓
Potential to involve ESS DEMAX ✓

6

Conclusions

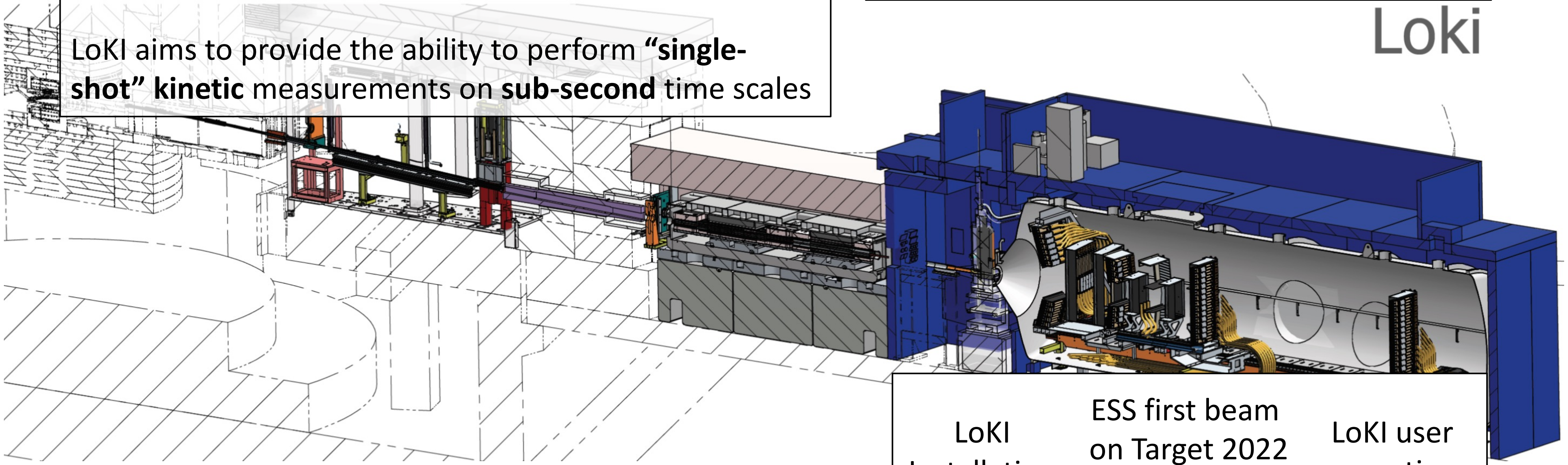
Conclusions

LoKI will have **high flux**, **wide simultaneous size range**, and a **flexible sample area**.

LoKI will enable the use of small beams, making **scanning experiments** & **microfluidics** routine.

LoKI aims to provide the ability to perform **"single-shot" kinetic** measurements on **sub-second** time scales

- High flux – up to 1×10^9 n/cm^2/s (at 5 MW)
- 8 + 10 m collimation
- 14 Hz or 7 Hz operation
- Up to 20 Å bandwidth
- Option for resolution enhancing choppers



Day 1 Performance (2 MW):

- Approx. 5x compared to D22 (LoKI at 14Hz)
- Approx. 20x SANS2D (LoKI at 7 Hz)

LoKI Installation 2021-22

ESS first beam on Target 2022

LoKI user operation 2023

Thanks to the LoKI team

(we are much happier than this photo suggests…)