

# Neutron Scattering @ ESS

(selected topics)

Wojciech Zając

# ESS – sept. 2020



World's brightest pulsed neutron source, one of the biggest and most advanced research infrastructures.  
ERIC since 2015

**Linear proton accelerator:**

- Energy: 2 GeV
- Current: 62.5 mA
- Pulse length: 2.86 ms
- Rep. rate: 14 Hz
- Average beam power: 5 MW
- Currently funded: 2 MW

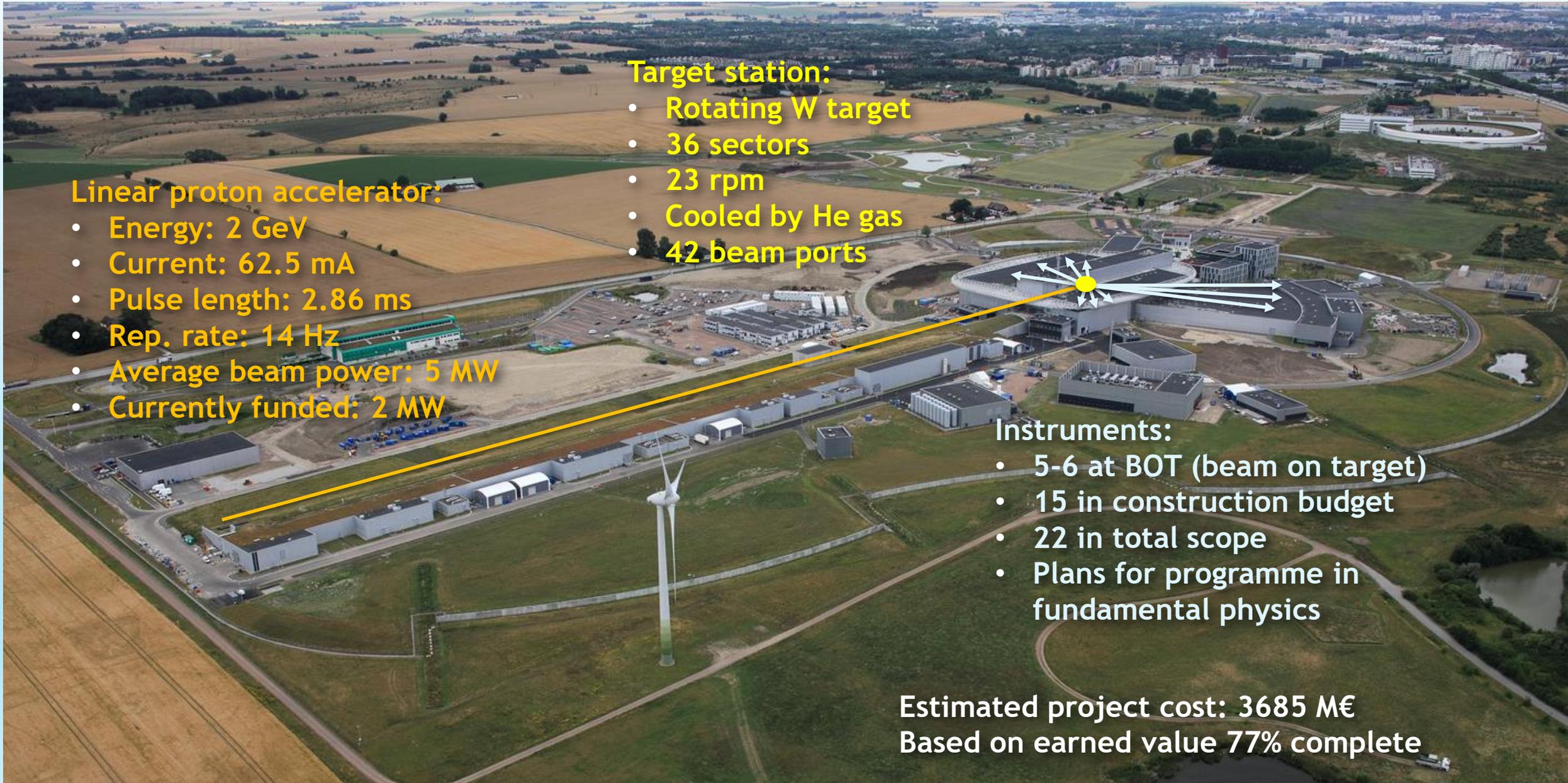
**Target station:**

- Rotating W target
- 36 sectors
- 23 rpm
- Cooled by He gas
- 42 beam ports

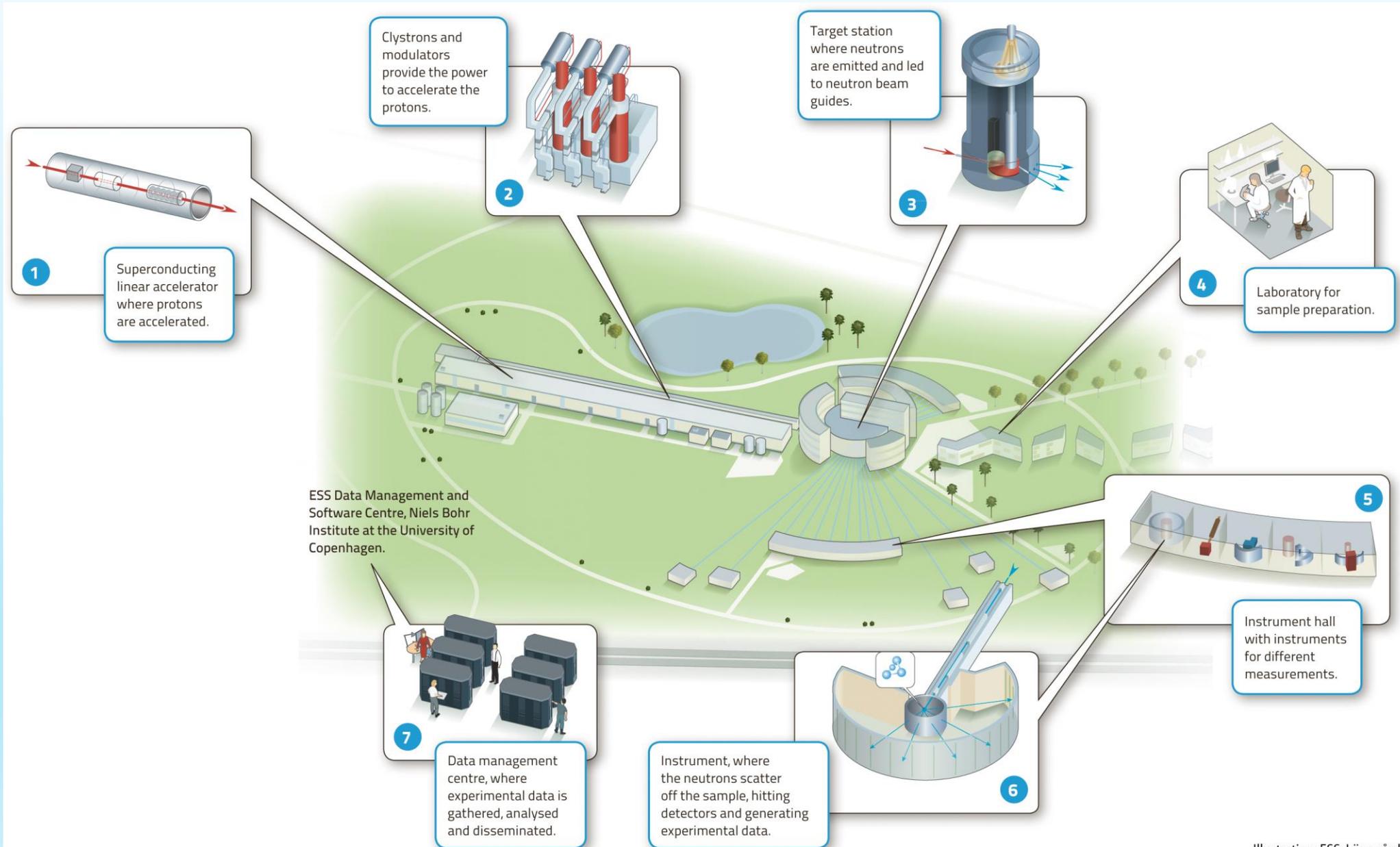
**Instruments:**

- 5-6 at BOT (beam on target)
- 15 in construction budget
- 22 in total scope
- Plans for programme in fundamental physics

Estimated project cost: 3685 M€  
Based on earned value 77% complete

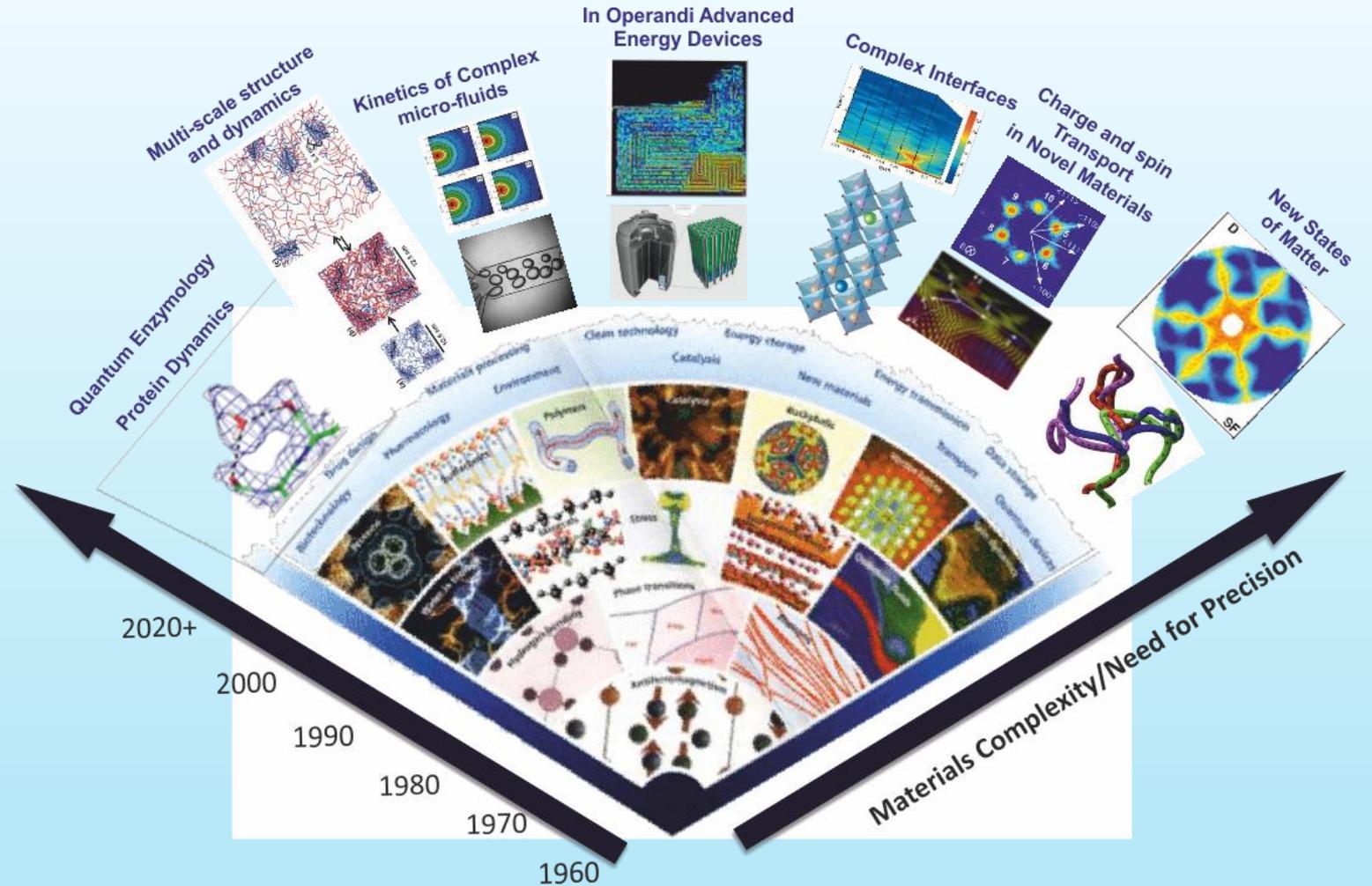


# ESS – schematic site layout



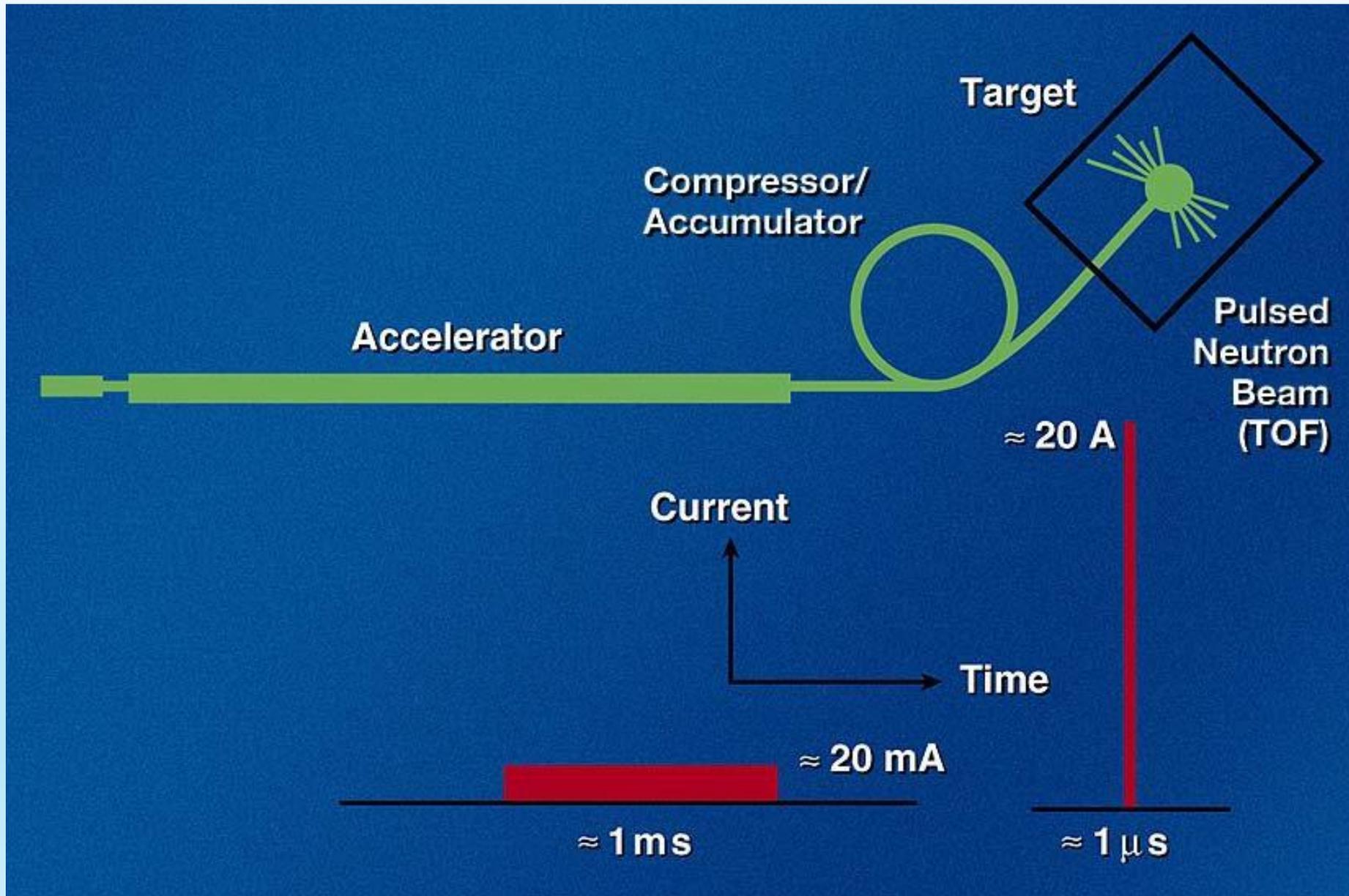
## ESS designed to meet the present and future research needs in:

- Physics
- Chemistry
- Materials sciences
- Engineering of modern machinery
- Energy production and storage
- Environmental sciences
- Life and health sciences



Poland contributes 1.8% of the ESS building budget

# What would we need for a shot-pulse source?



# ESS – how it works

1 Protons are generated in the ion source

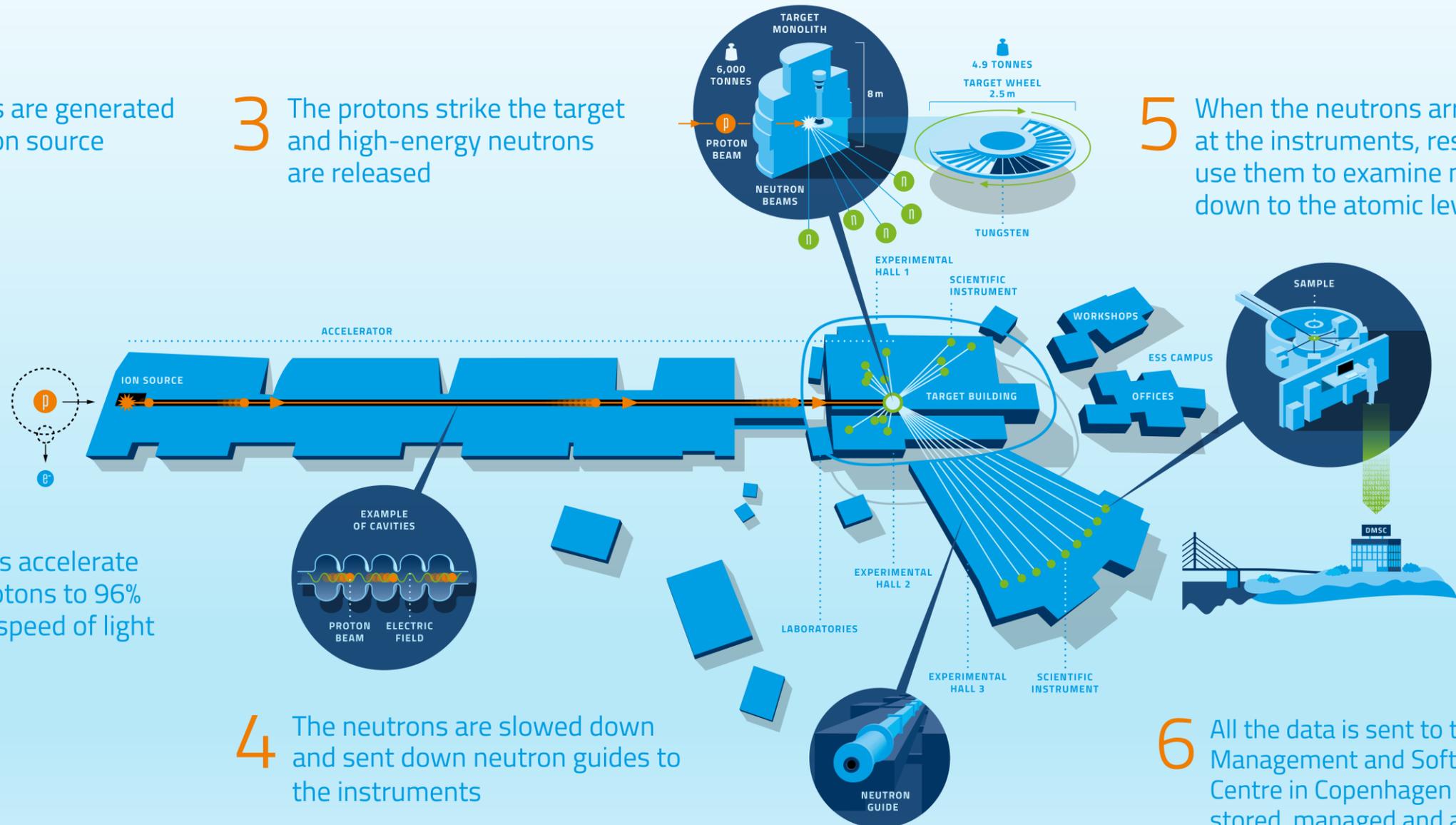
3 The protons strike the target and high-energy neutrons are released

2 Cavities accelerate the protons to 96% of the speed of light

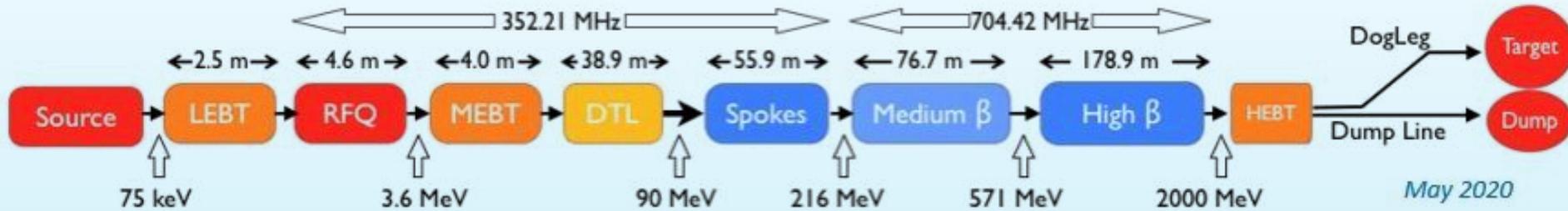
4 The neutrons are slowed down and sent down neutron guides to the instruments

5 When the neutrons arrive at the instruments, researchers use them to examine matter down to the atomic level

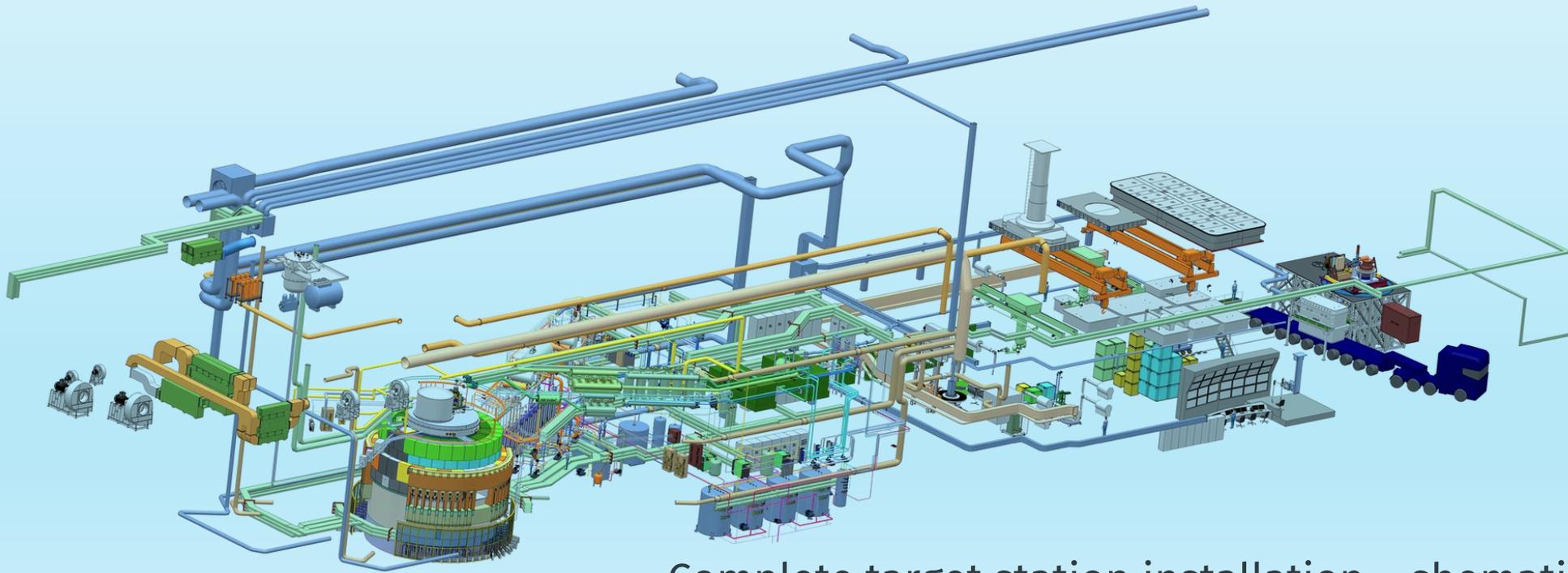
6 All the data is sent to the Data Management and Software Centre in Copenhagen to be stored, managed and analysed with the researchers



# ESS – how it works

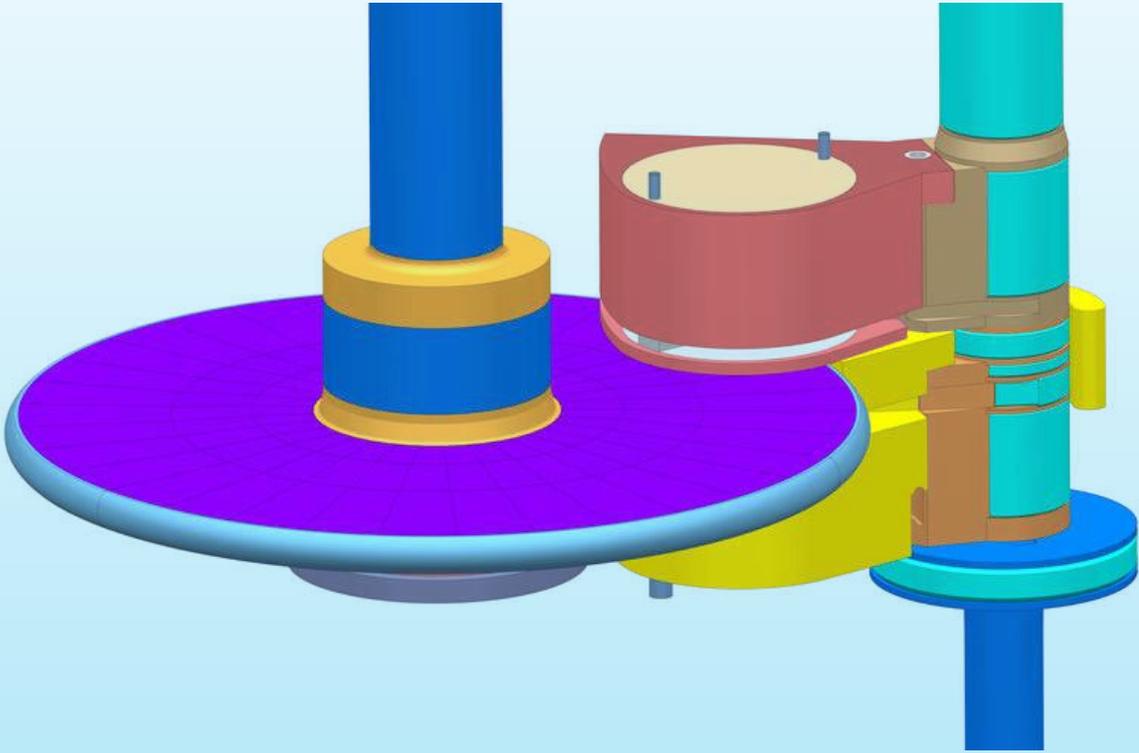
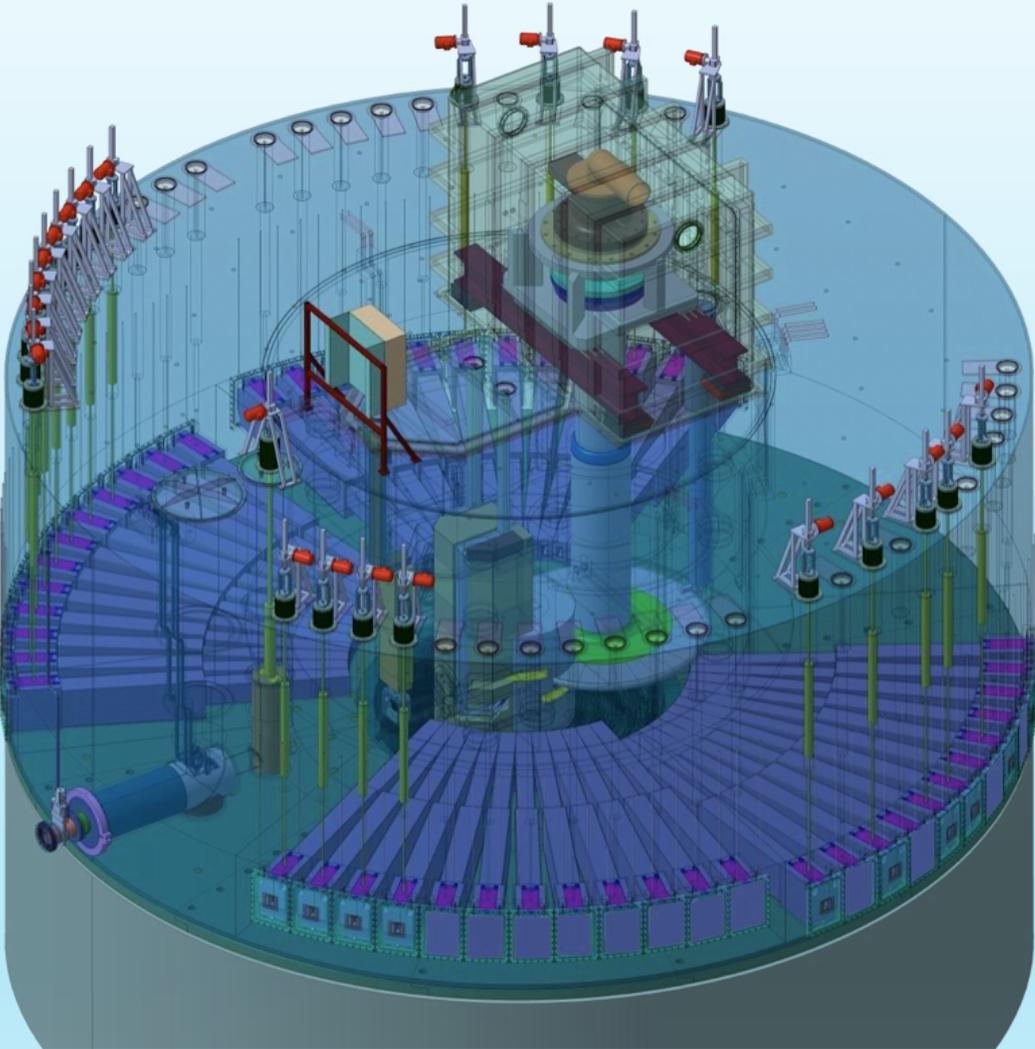


Linac delivers 2–2.5 GeV protons at the target



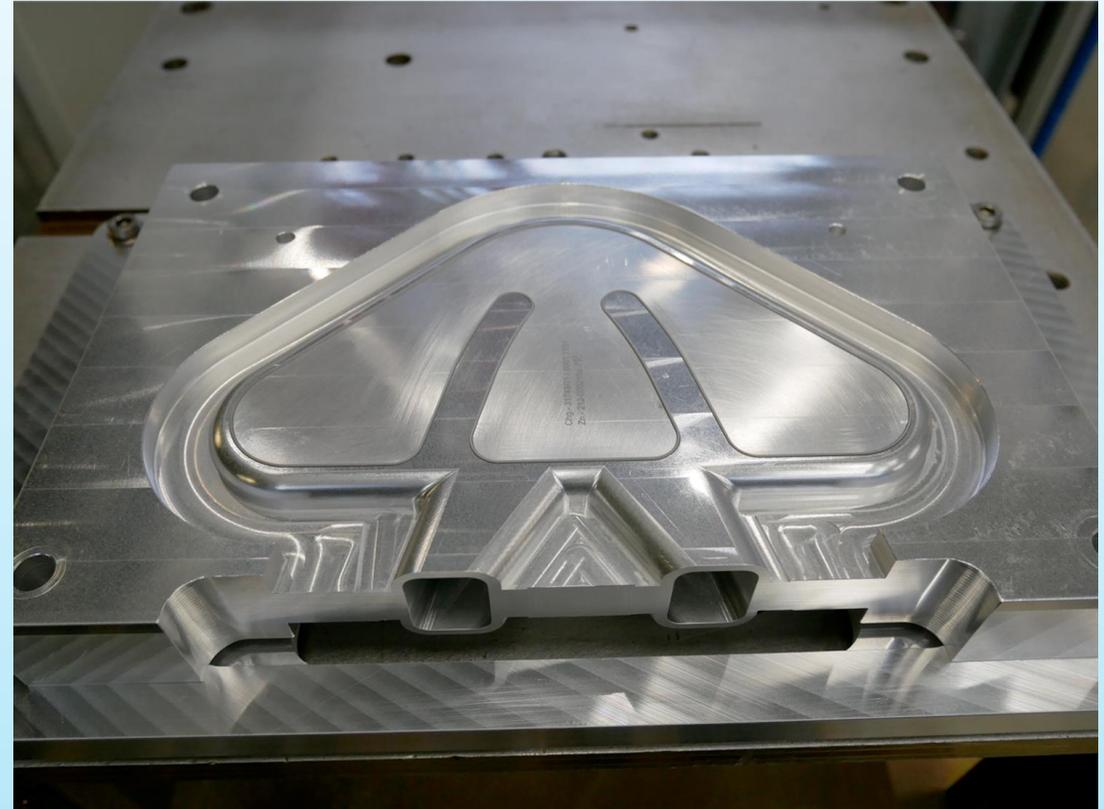
Complete target station installation – schematic drawing

# ESS – target station



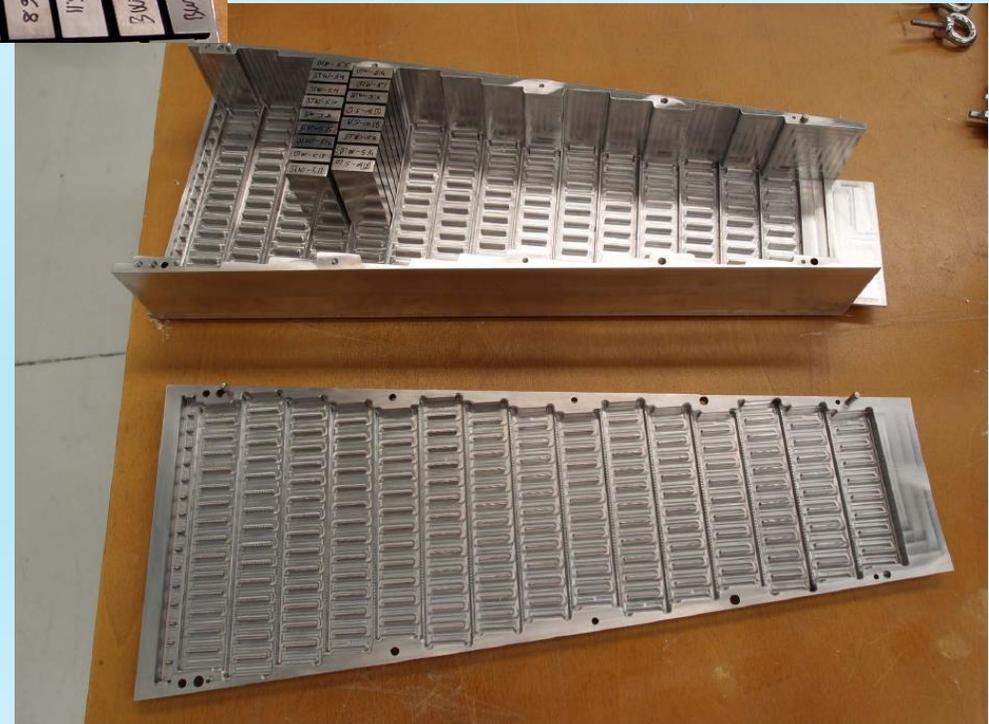
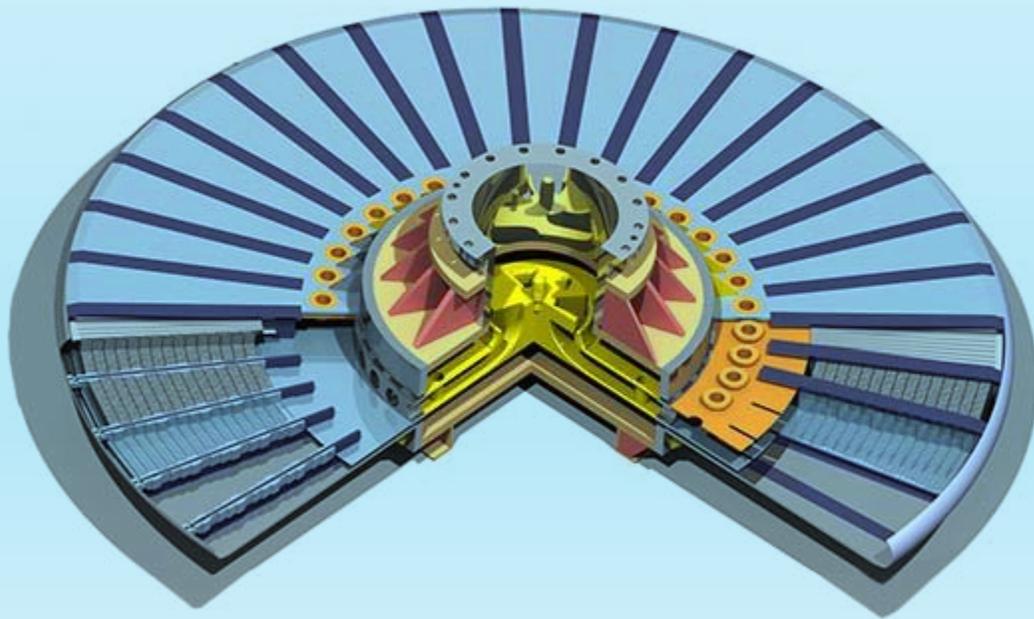
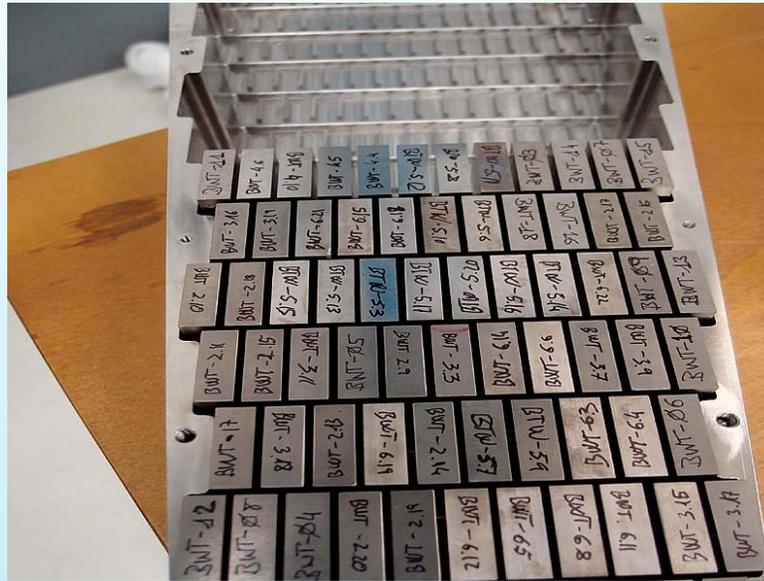
Target station – schematic drawing

# ESS – target wheel and the moderator housing

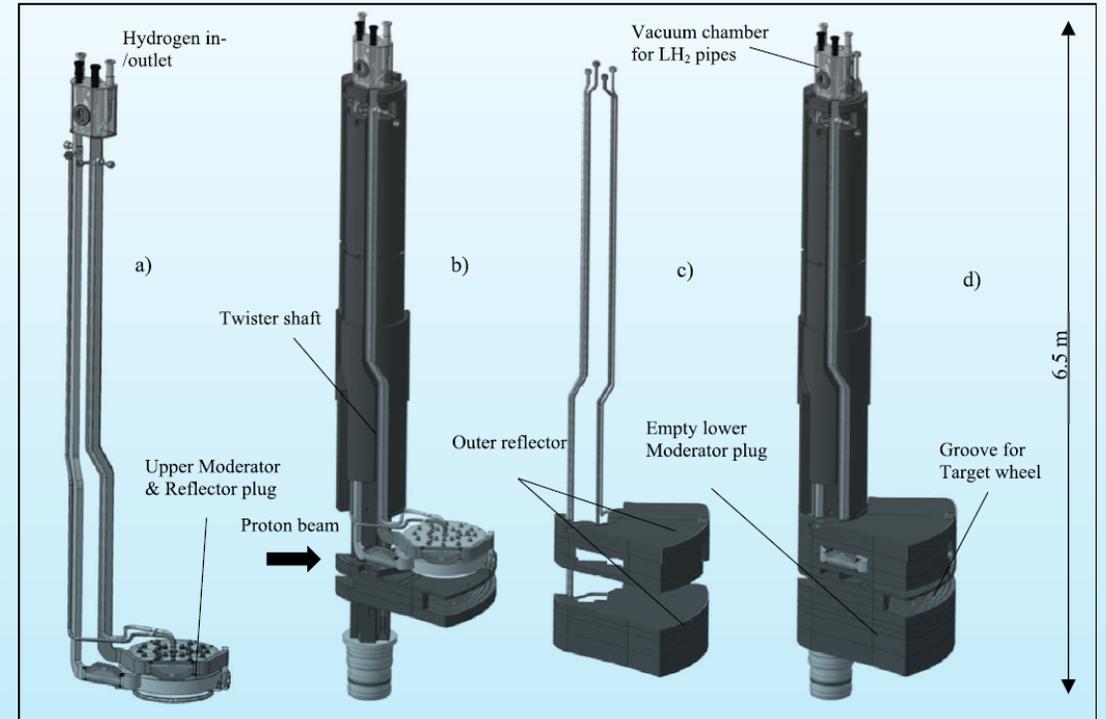


# ESS – target monolith

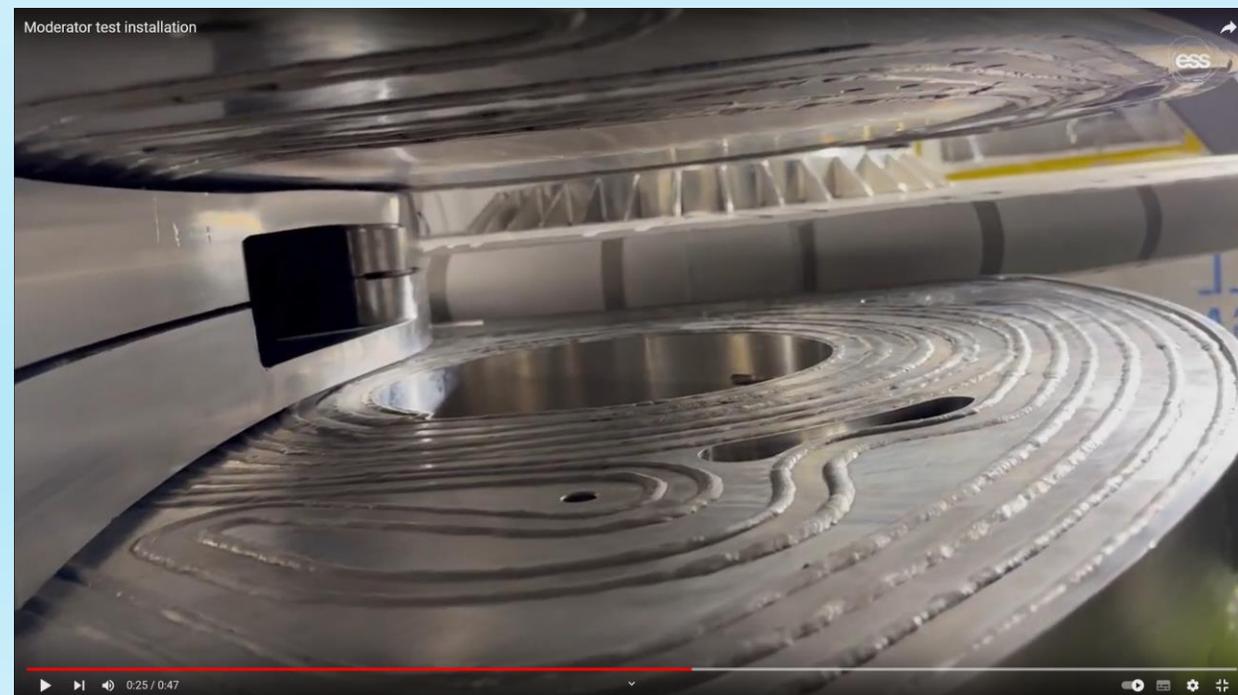
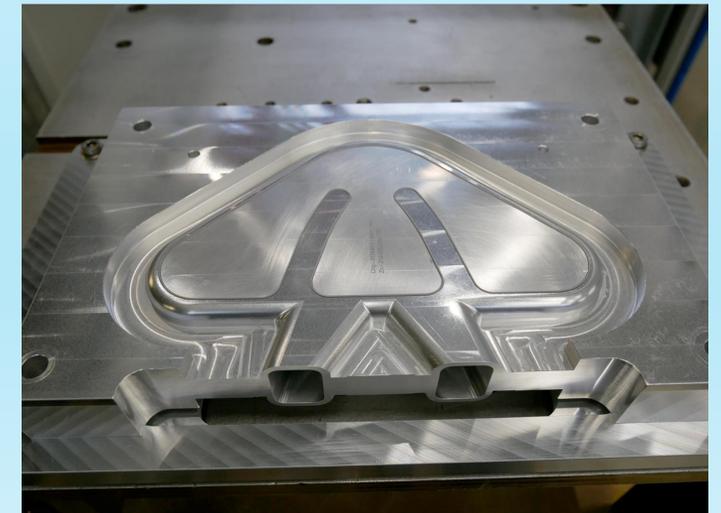
7000 tungsten bricks ready for mounting on the ESS target wheel prototype.



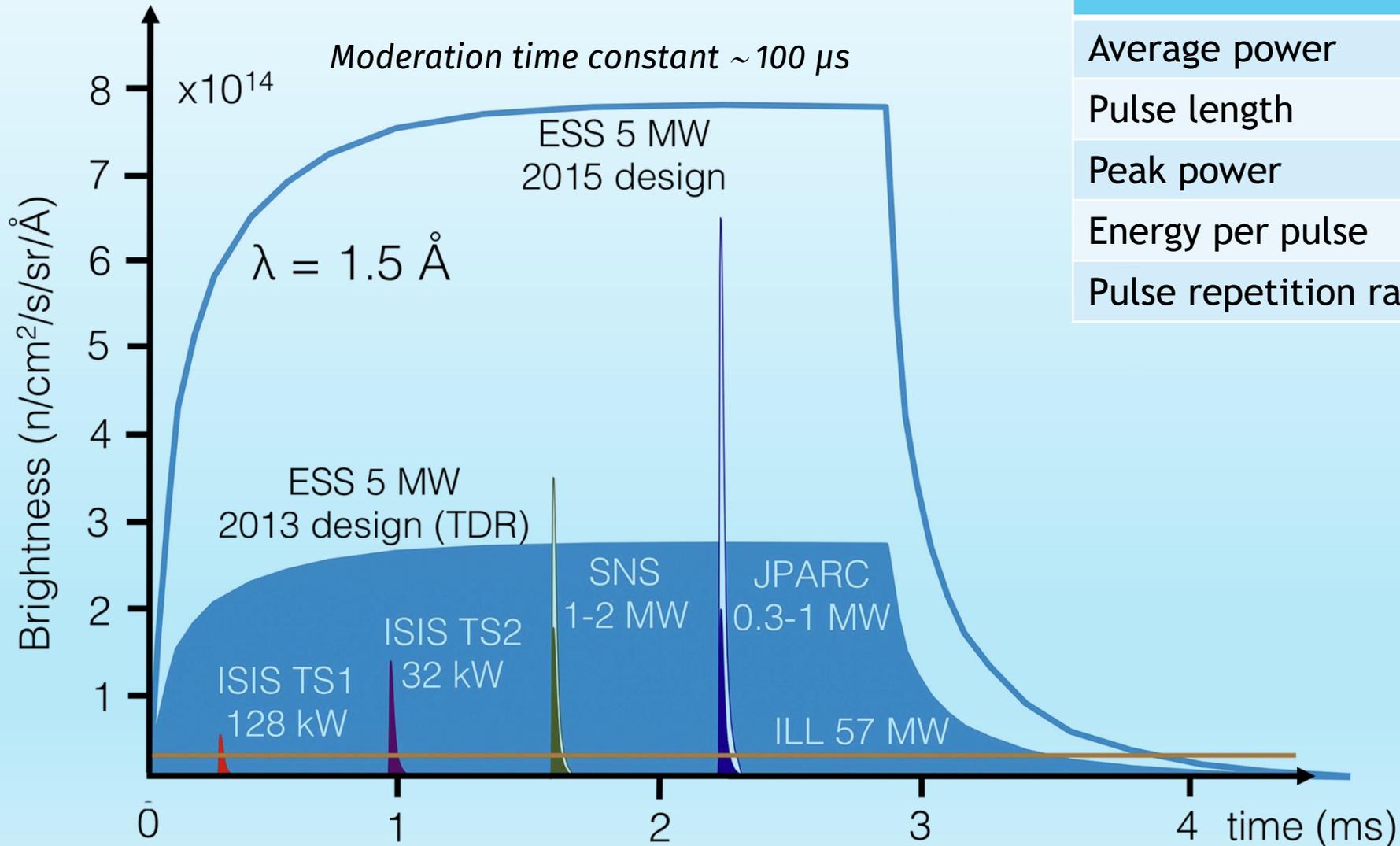
# ESS moderators



„Butterfly”  
moderator



# ESS – the long pulse source

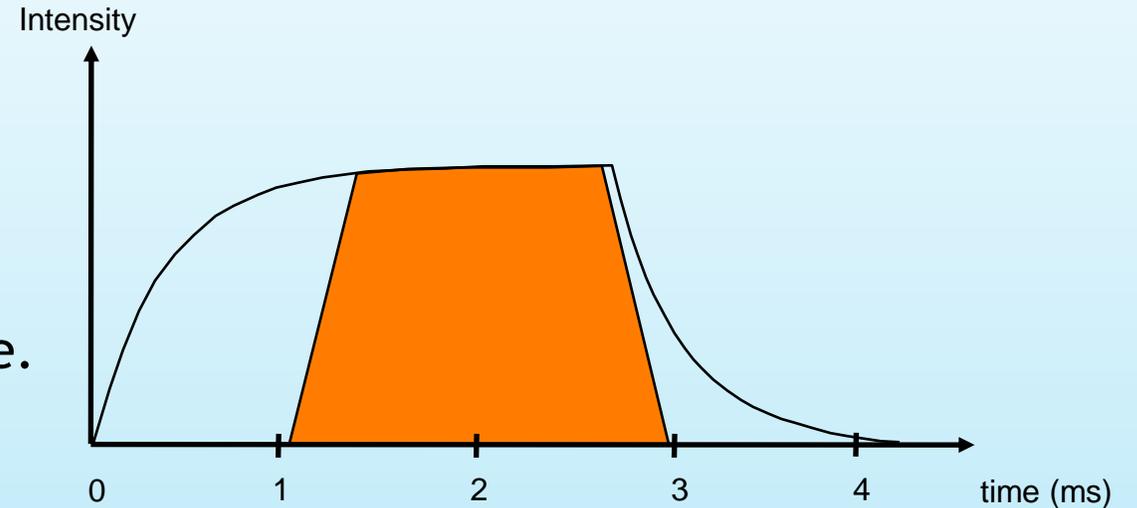


	SNS	ESS
Average power	1.4 MW	5 MW
Pulse length	695 ns	2.86 ms
Peak power	34 GW	125 MW
Energy per pulse	24 kJ	357 kJ
Pulse repetition rate	60 Hz	14 Hz

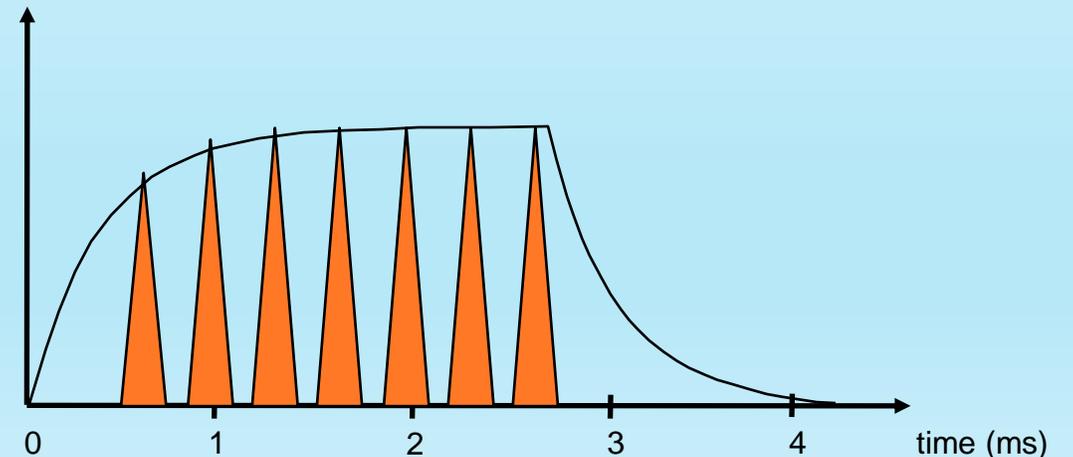
Time-averaged  
brightness:  
ESS  $\sim$  ILL  
Peak brightness:  
ESS  $\sim 30 \times$  ILL

# ESS – the long pulse source

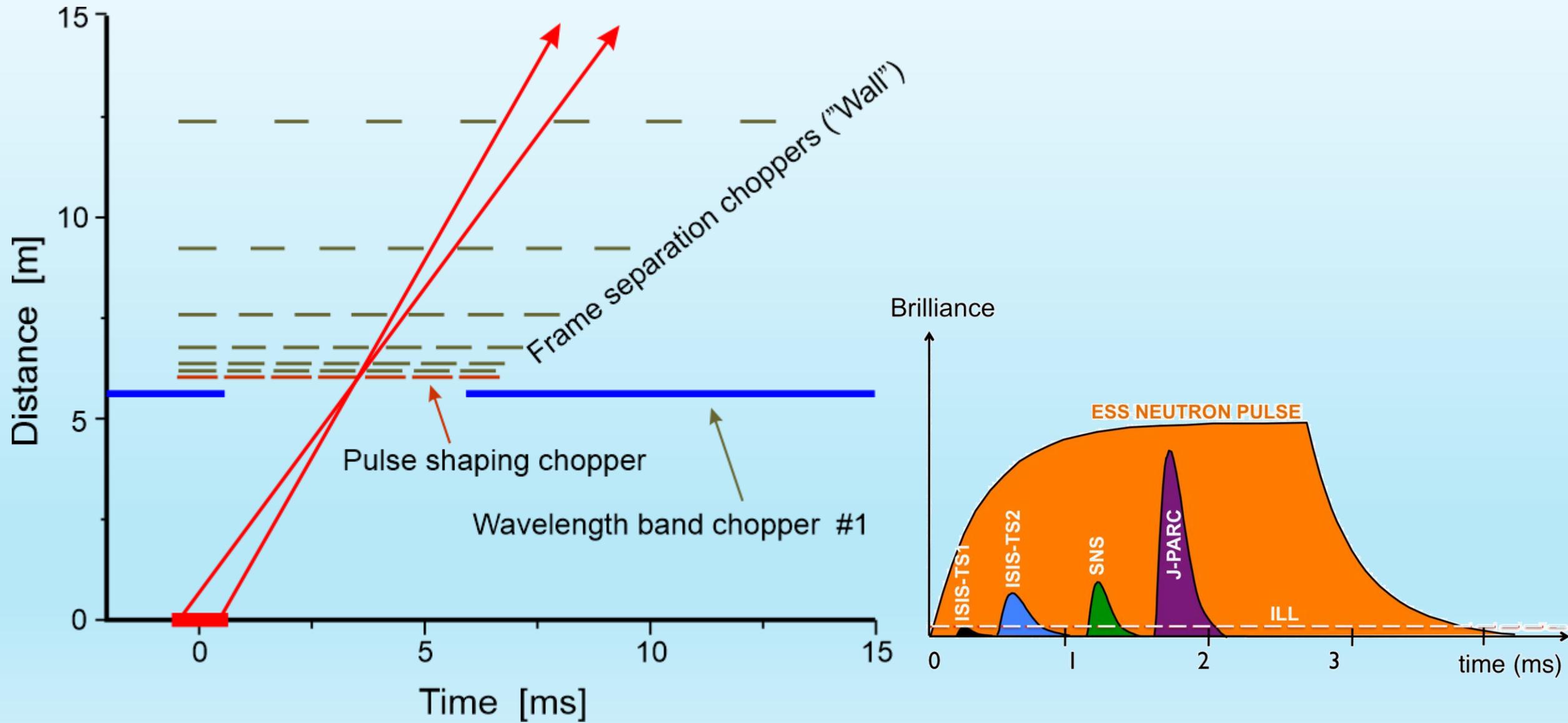
**Use as much as possible of the whole pulse:**  
Good for low wavelength resolution instruments.  
SANS, Reflectometry, single crystal diffraction.  
Estimated gains **10–100 times** the currently available.



**Cut the long pulse into smaller pulses:**  
Good for higher wavelength resolution instruments  
Diffraction, cold/thermal spectrometers.  
Long Instruments (80-100 m)  
Estimated gains **10-30 times** than currently available.  
Thermal gains lower.

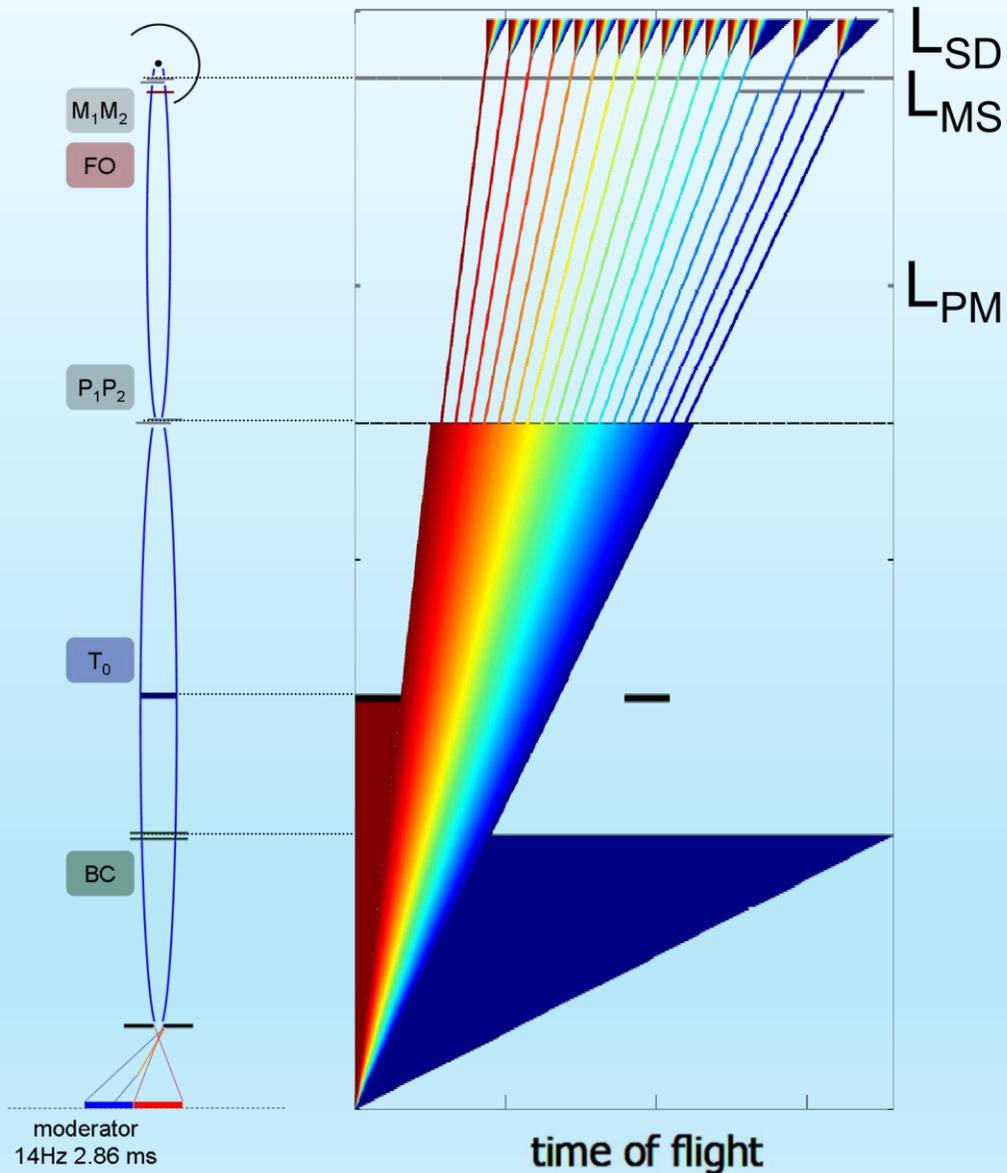


# ESS – secondary pulse shaping (Mezei)



# ESS – repetition rate multiplication

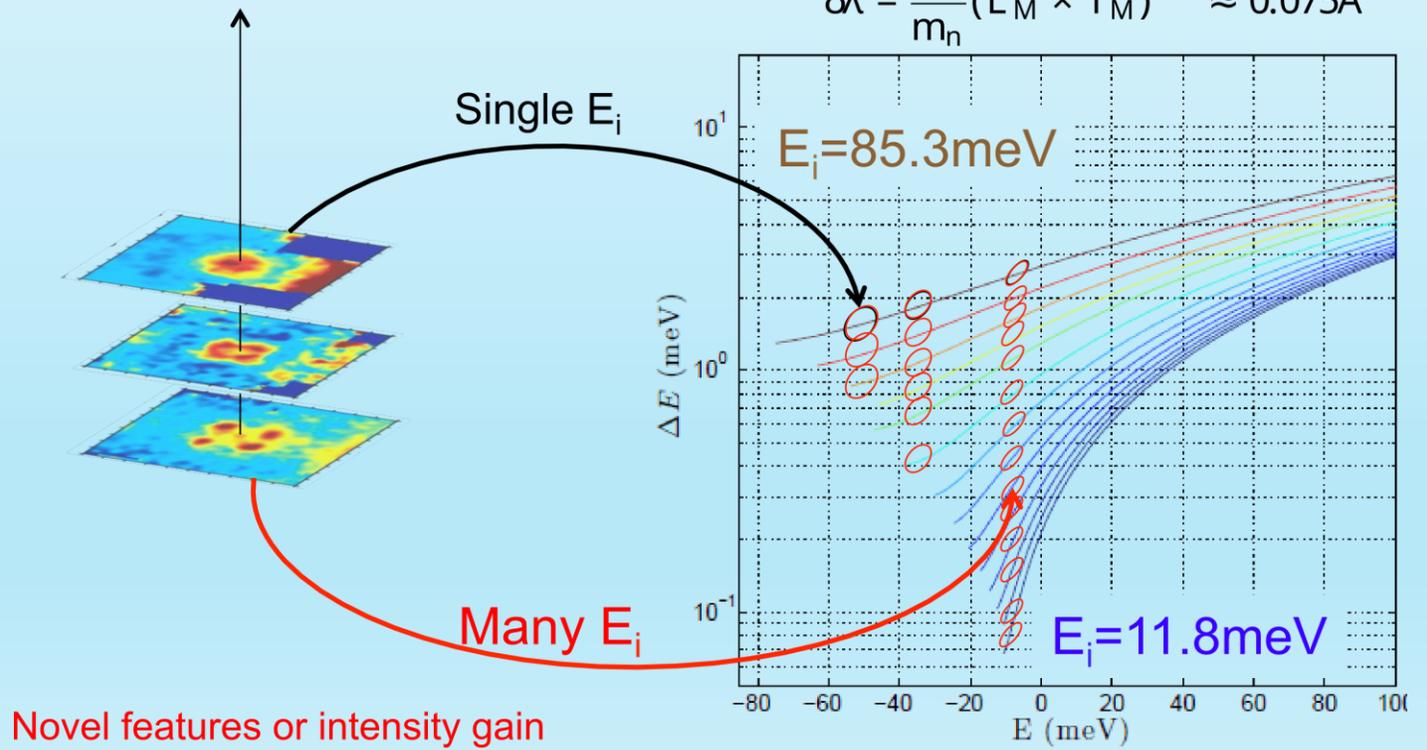
(from T-REX original proposal)



$$L = 155\text{m}, L_M = 150\text{m}$$

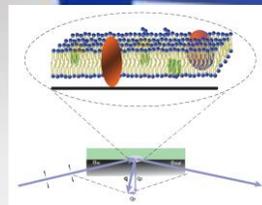
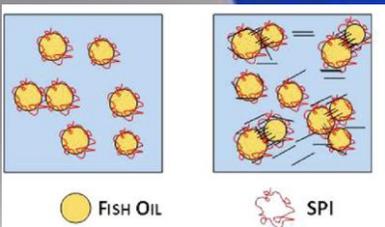
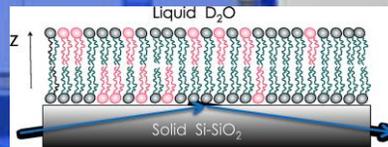
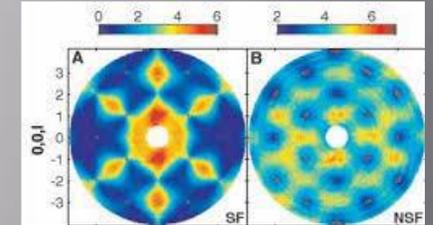
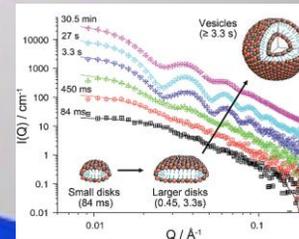
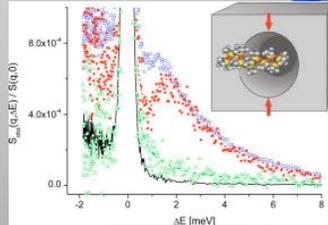
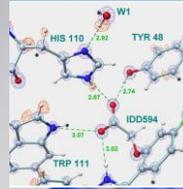
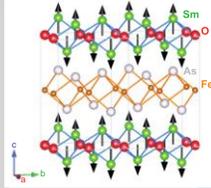
$$\Delta\lambda = \frac{h}{m_n} (L \times 14\text{Hz})^{-1} \approx 1.8\text{\AA}$$

$$\delta\lambda = \frac{h}{m_n} (L_M \times f_M)^{-1} \approx 0.075\text{\AA}$$



## Instrument classes

- Imaging (ODIN)
- SANS (LoKI)
- Reflectometers (Estia)
- Spectrometers (BIFROST)
- Diffractometers (NMX, DREAM)



The first 15 instruments at the ESS

ODIN  
DREAM

VESPA

SKADI

ESTIA

FREIA

LoKI

NMX

BEER

C-SPEC

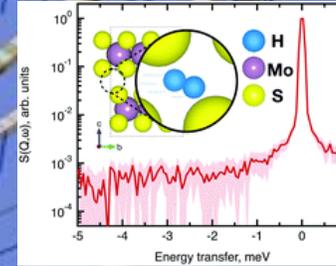
BIFROST

MIRACLES

MAGIC

T-REX

HEIMDAL



# ESS instrument suite

## Large-Scale Structures

ODIN imaging     

SKADI GP-SANS    

LOKI Broadband SANS  

Surface Scattering    

FREIA Hor. Refl.   

ESTIA Ver. Refl.    

HEIMDAL Pow. Diffr.    

DREAM Pow. Diffr.    

## Diffraction

Monochromatic Powder Diffractometer   

BEER Eng. Diffr.   

Extreme Conditions Diffractometer    

MAGIC Magn. Diffr.  

NMX Macromol. Diffr.  

## Spectroscopy

CSPEC ColdChopSp   

VOR BroadbandSp    

T-REX ThChopSpec   

BIFROST Xana Spec    

VESPA Vibr.Spec.   

MIRACLES BckScatt   

High-Resolution Spin-Echo    

Wide-Angle Spin-Echo    

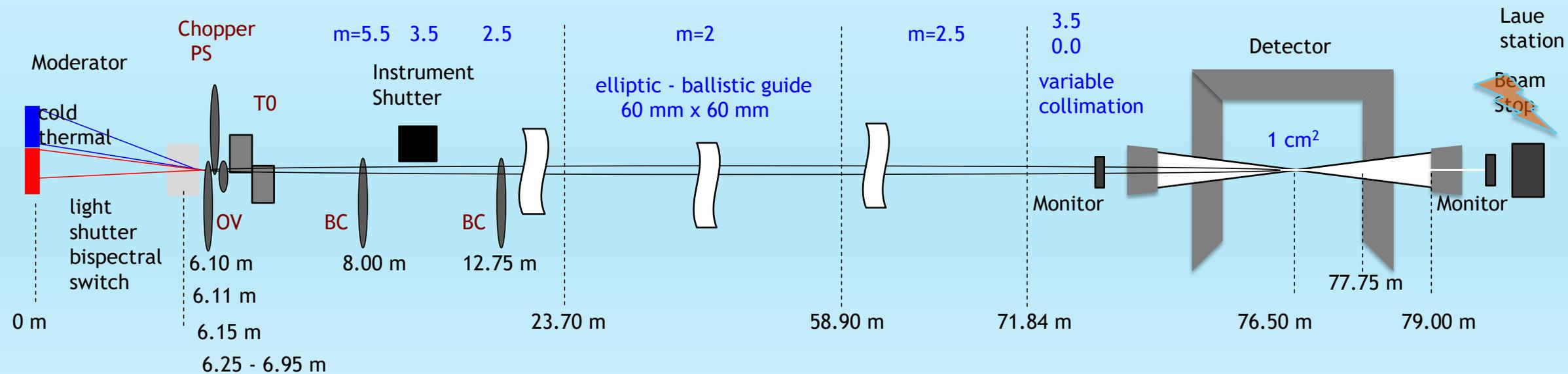
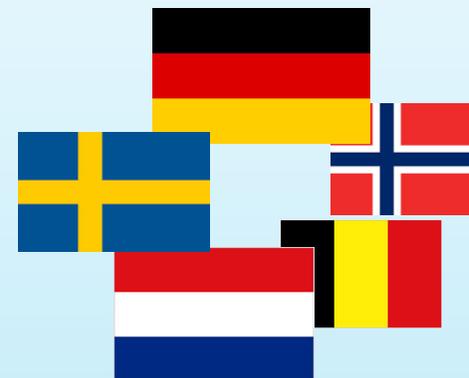
Fundamental & Particle Physics 

15 approved  
8 at «Day 0»

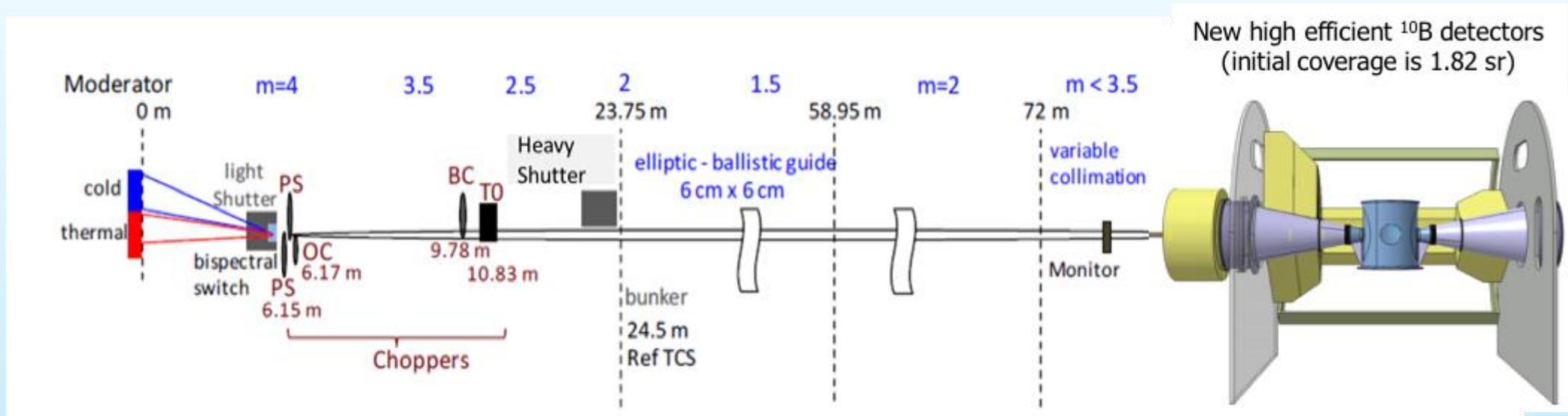
	life sciences		magnetism & superconductivity
	soft condensed matter		engineering & geo-sciences
	chemistry of materials		archeology & heritage conservation
	energy research		fundamental & particle physics

# DREAM – Bispectral Powder Diffractometer

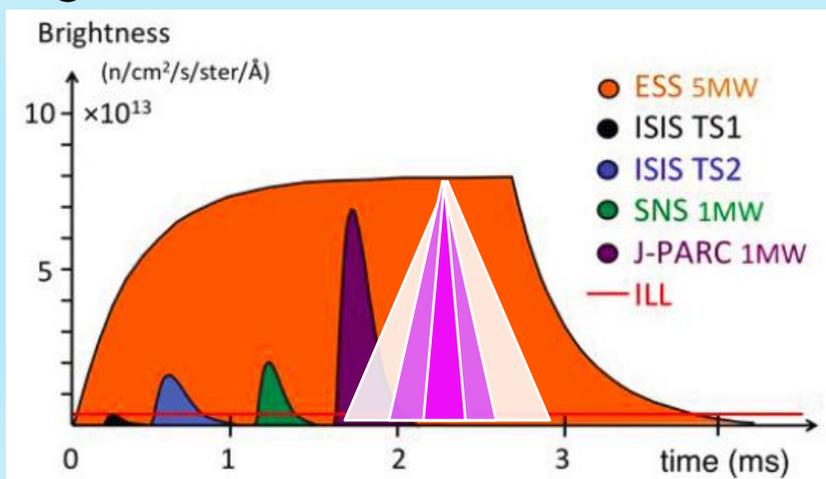
## Diffraction Resolved by Energy and Angle Measurements



# DREAM – Bispectral Powder Diffractometer



## Brightness



*pulse shaping*

75 m length

bandwidth includes thermal and cold peak

thermal spectrum gives  $Q_{\text{max}} < 25 \text{ \AA}^{-1}$

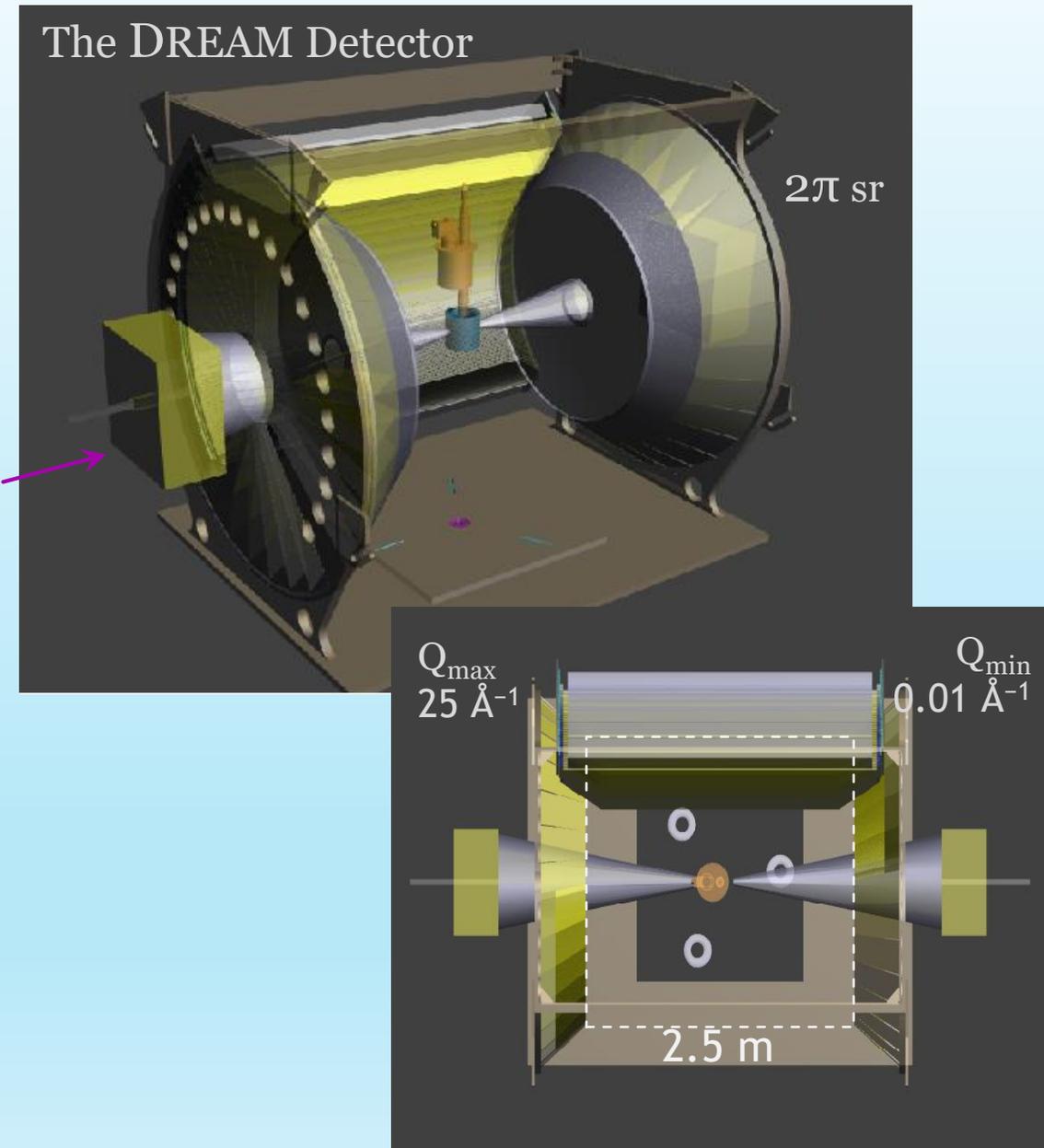
high flexibility in trading resolution vs intensity

ideal peak shape

using the intense cold spectrum with best ever resolution

# DREAM – Bispectral Powder Diffractometer

The DREAM Detector



VITESS

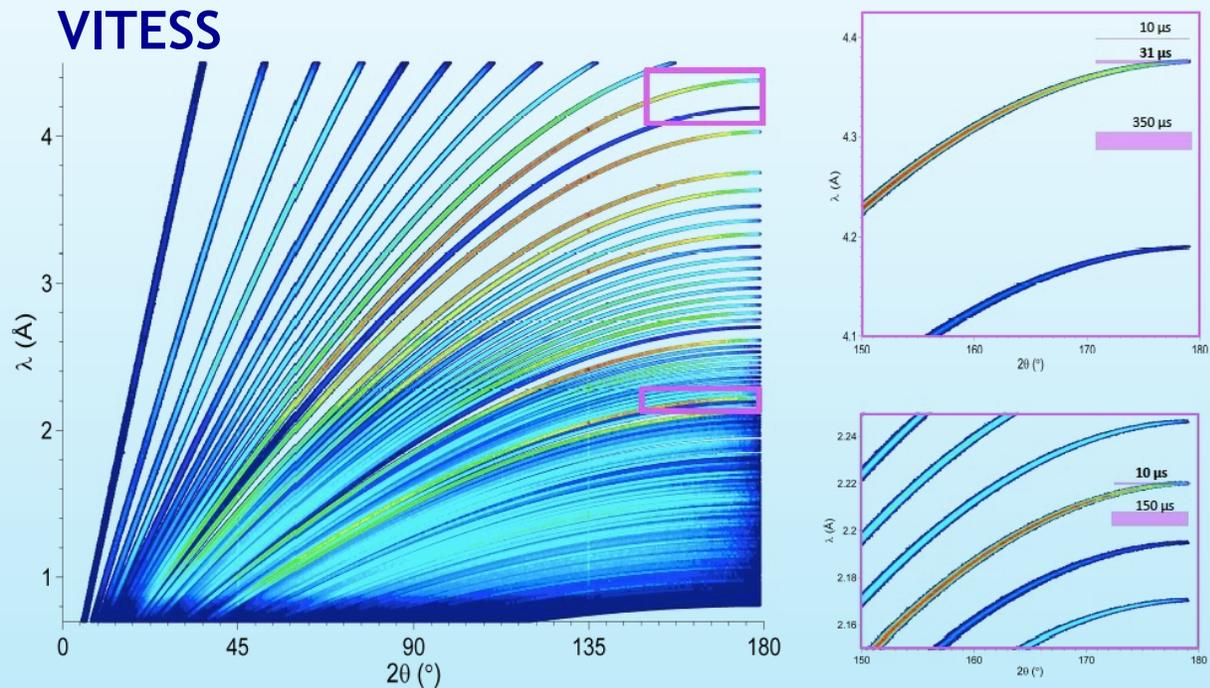
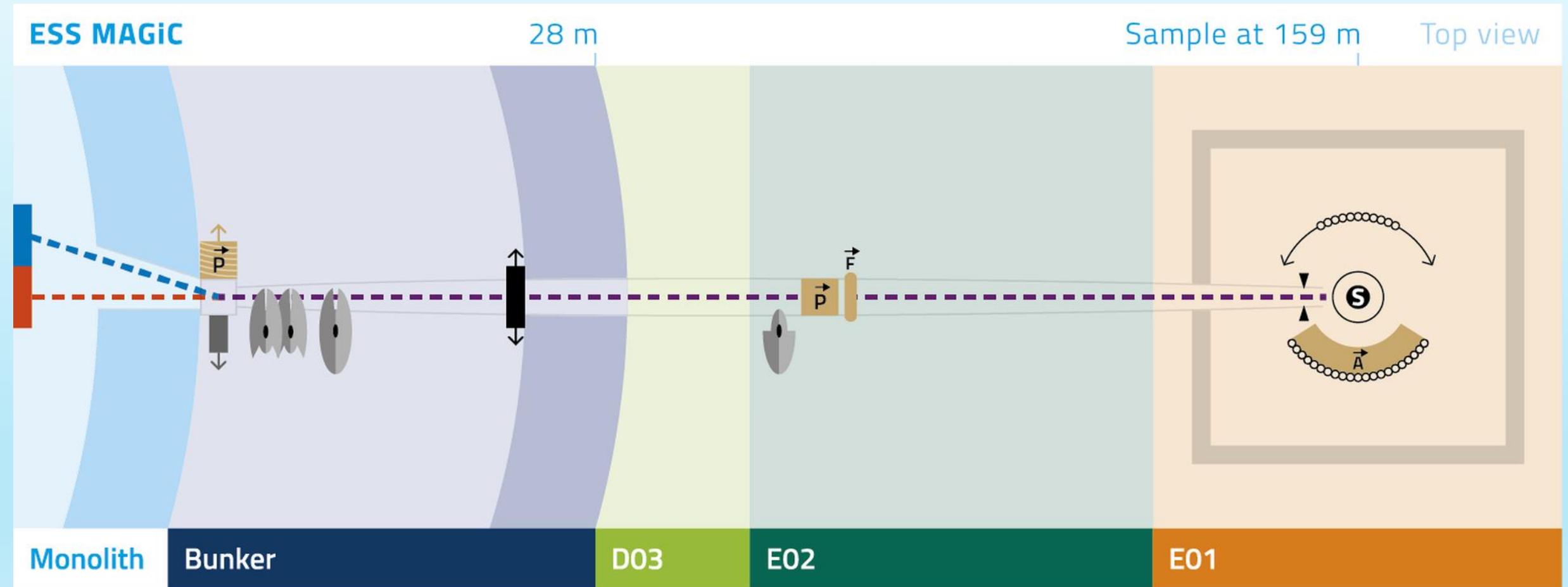


Fig. 5 Diffraction diagram of a reference sample ( $0.4 \text{ cm}^3 \text{ Na}_2\text{Ca}_3\text{Al}_2\text{F}_{14}$ ) in high resolution mode (left). In backscattering, the asymptotic limit is essentially determined by the time resolution, see enlarged regions (right)

# MAGiC – Magnetism Single-Crystal Diffractometer

## Polarized time-of-flight single-crystal diffractometer



# MAGiC – Magnetism Single-Crystal Diffractometer

The magnetic moment is a vector



Usually intensities are only measures of scalar products.

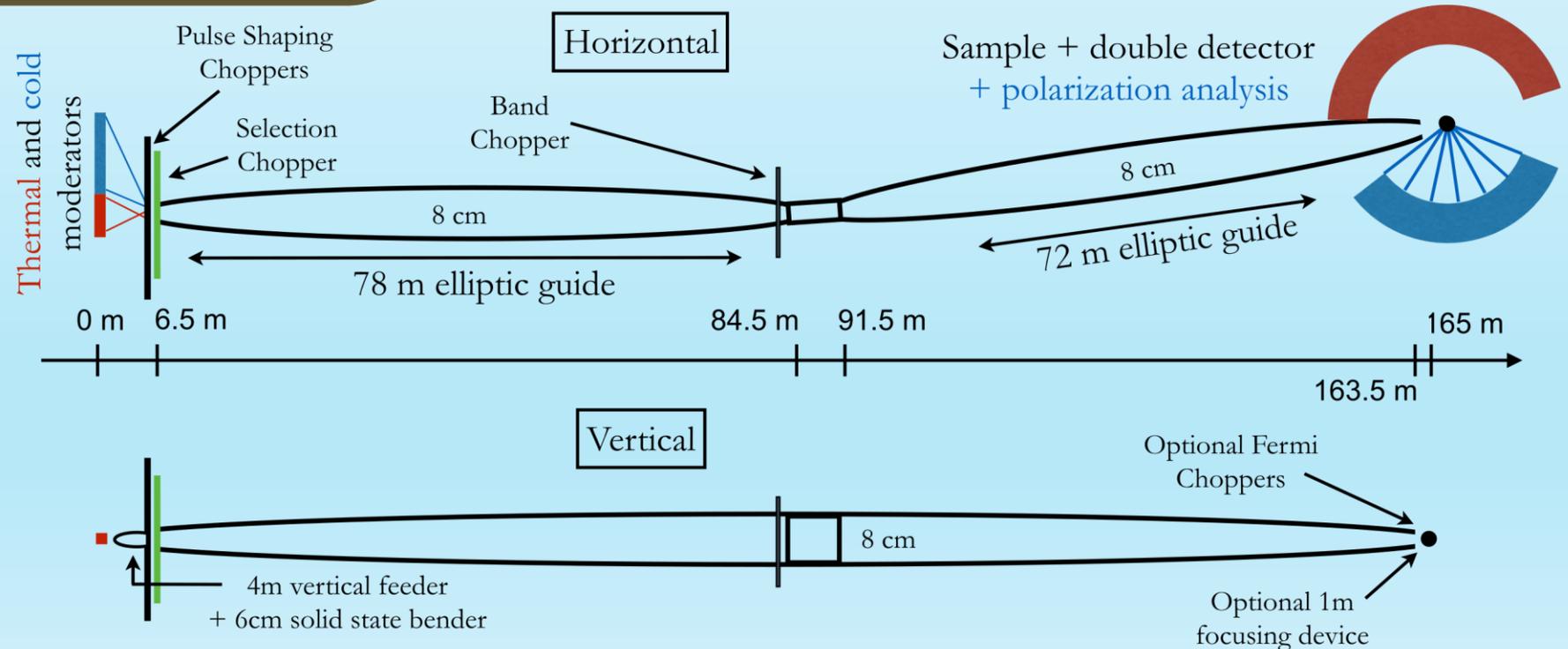
The neutron dipolar interaction probes magnetic moments perpendicular to the scattering vector

$$\vec{S}_{\perp\vec{Q}} \cdot \vec{S}'_{\perp\vec{Q}}$$

**Polarized neutrons** measure vector properties,

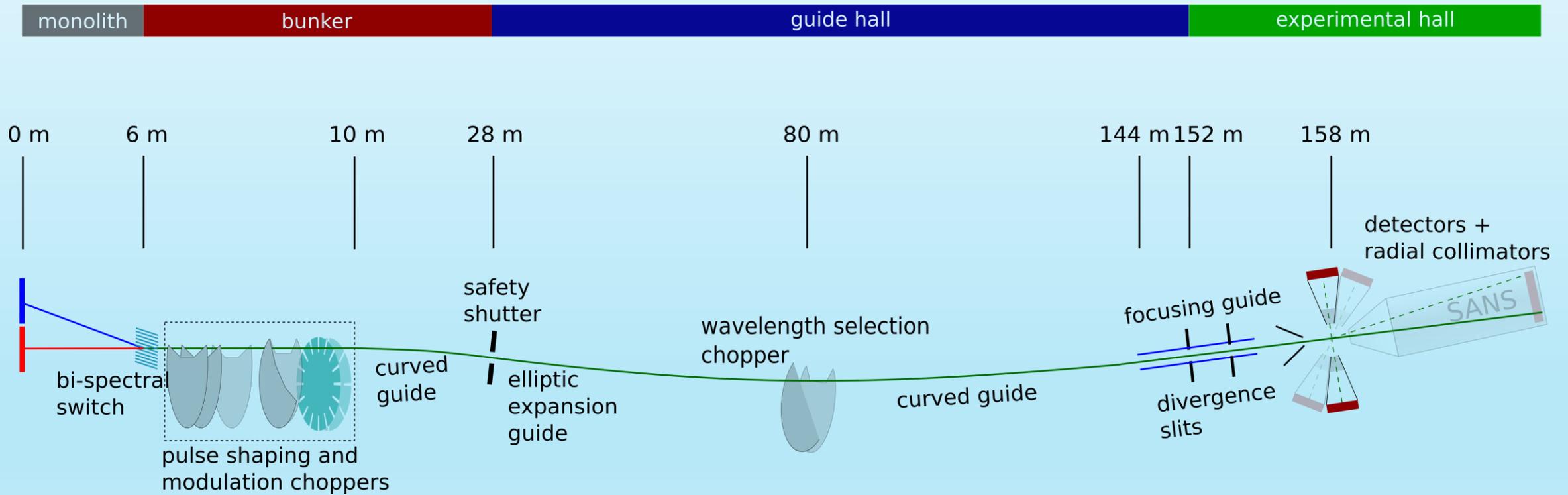
vector products and vector directions

$$\vec{S}_{\perp\vec{Q}} \times \vec{S}'_{\perp\vec{Q}}$$

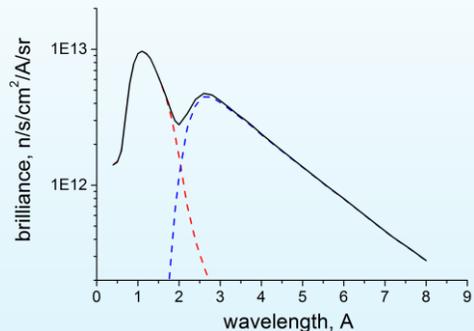


# BEER – Engineering Diffractometer

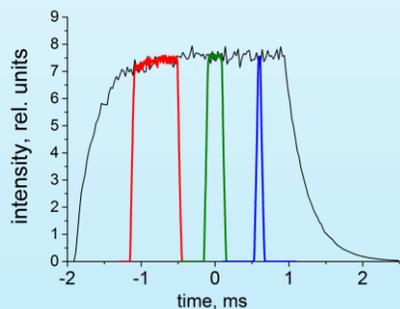
## Beamline for European Engineering Materials Research



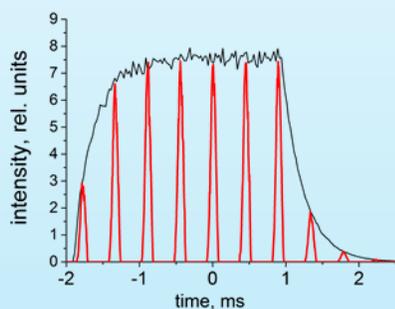
## bi-spectral source



## chopper system for wide range of resolutions



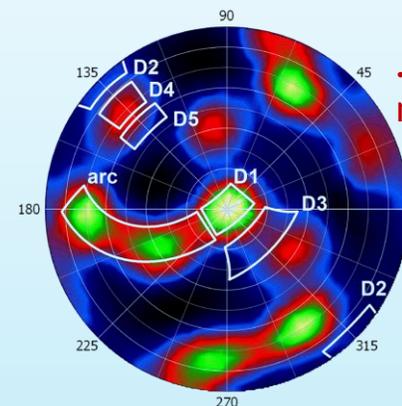
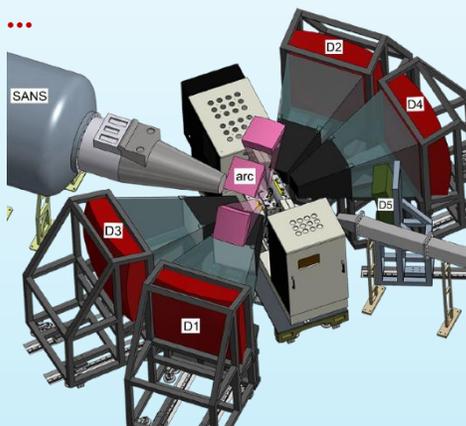
pulse shaping



pulse modulation

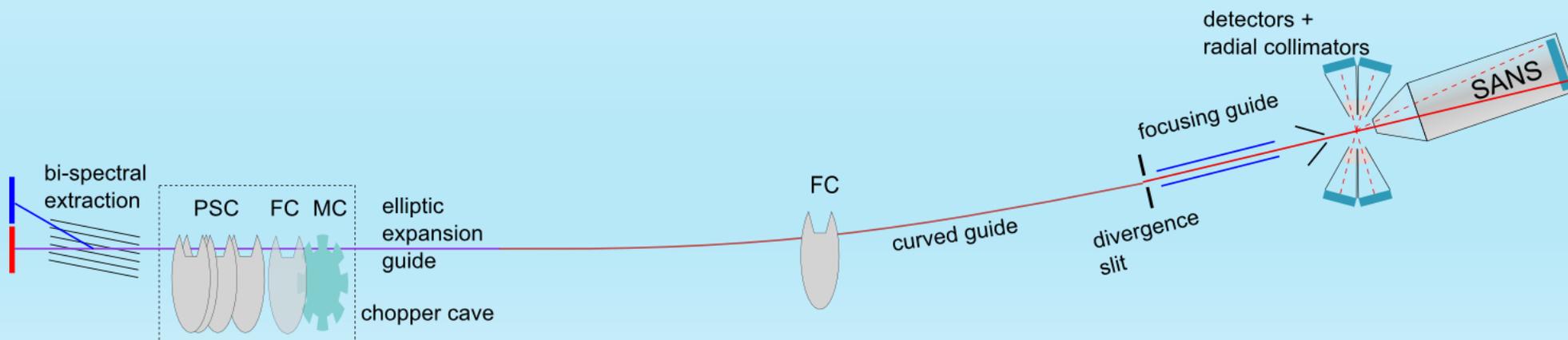
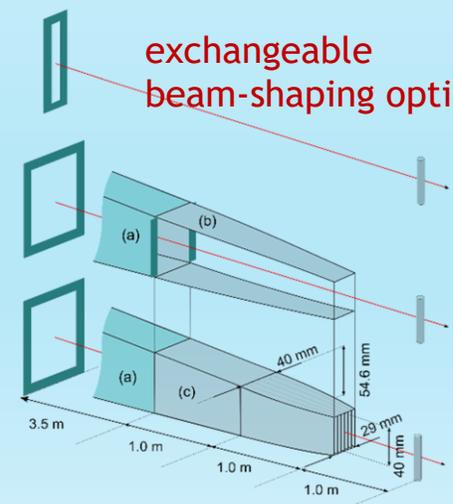
# BEER – Engineering Diffractometer

retractable detector banks allowing for large sample environment

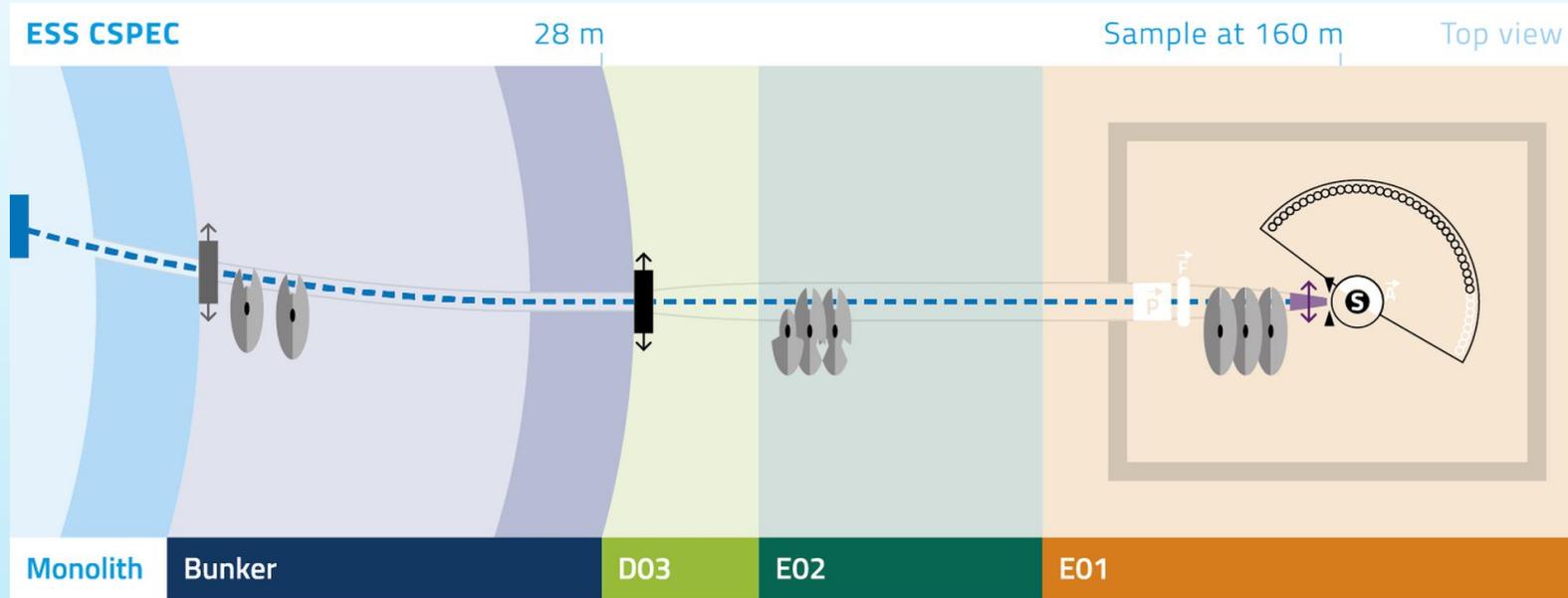


... and texture measurements

## exchangeable beam-shaping optics

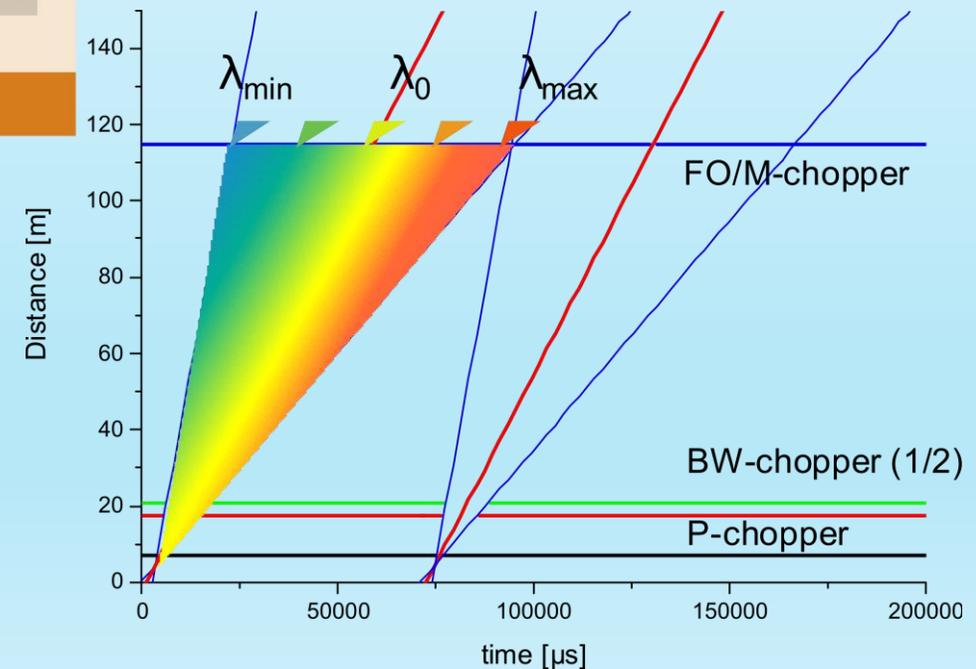


# CSPEC – Cold Chopper Spectrometer



**CSPEC** will be used in a wide variety of scientific applications, spanning the life sciences, functional materials and chemistry. *Its key capability is to follow kinetic events in situ or in operando, enabled by very high flux.*

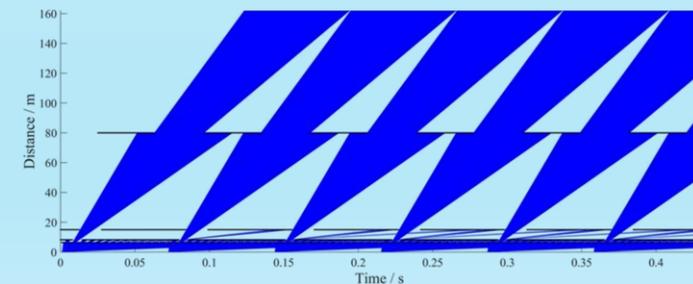
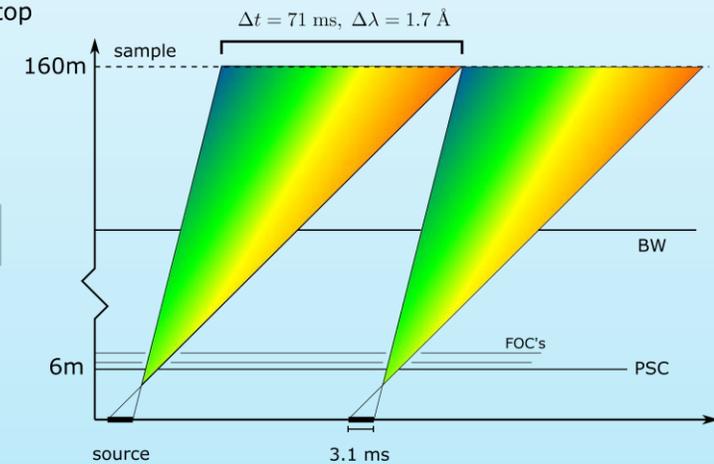
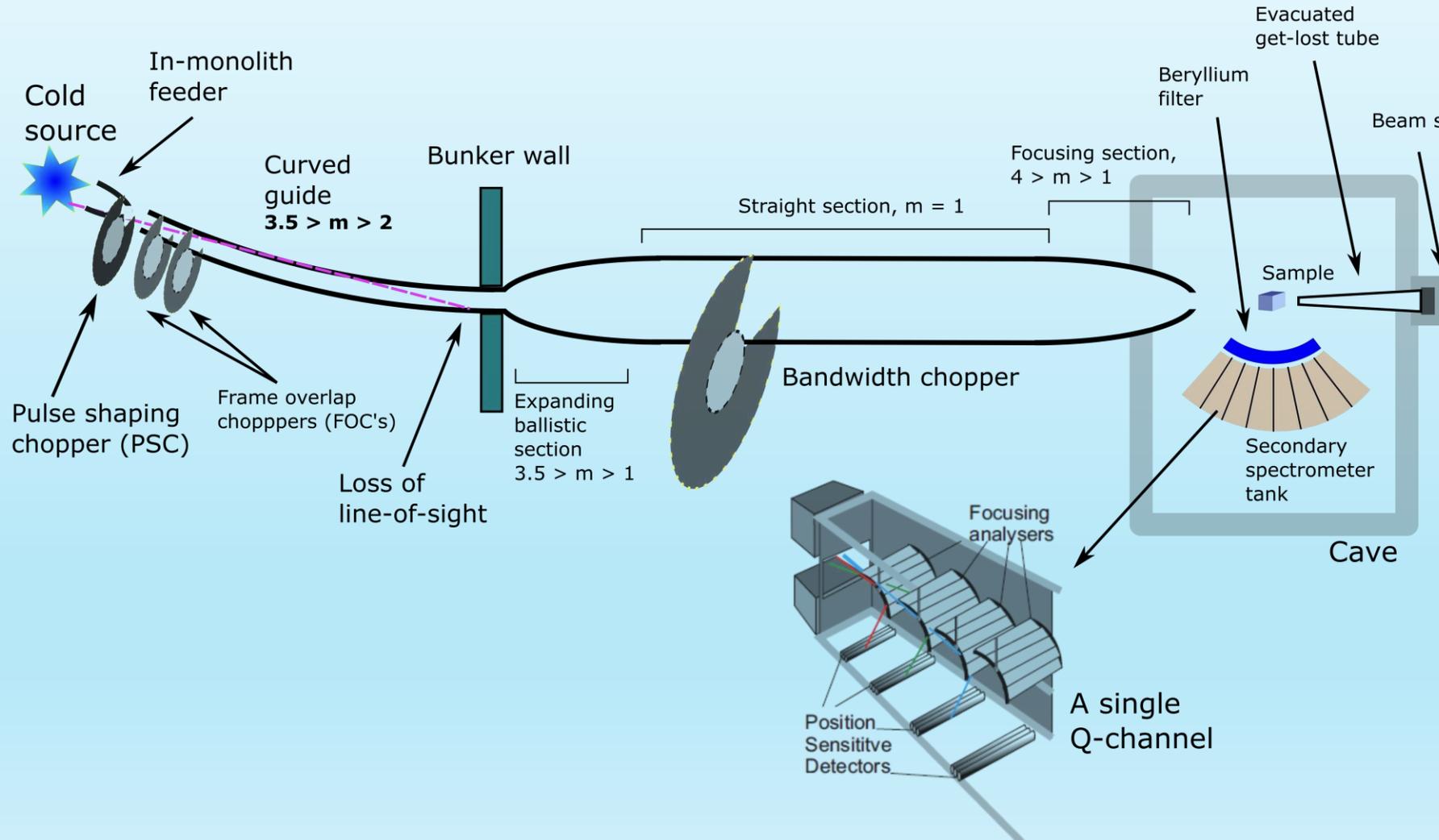
**CSPEC** is a direct geometry time of flight spectrometer developed as a German/French collaboration between FRM II and LLB.



# BIFROST – Extreme Environment Spectrometer

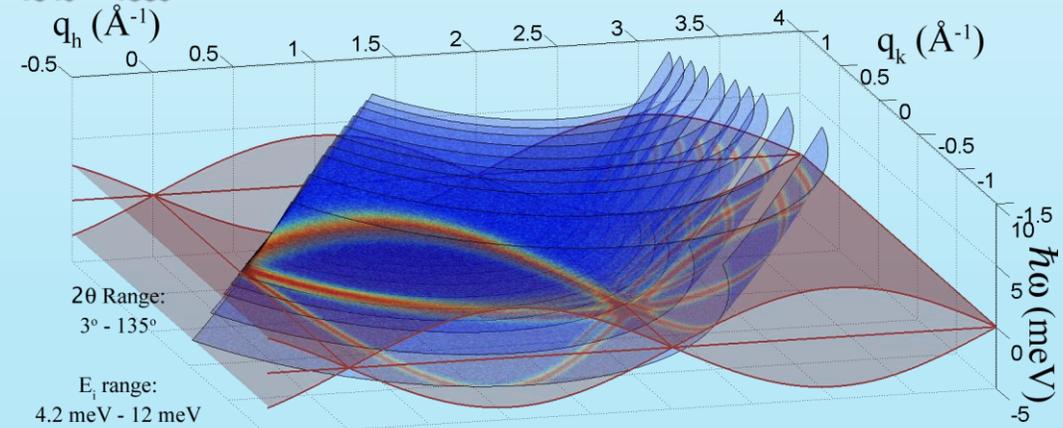
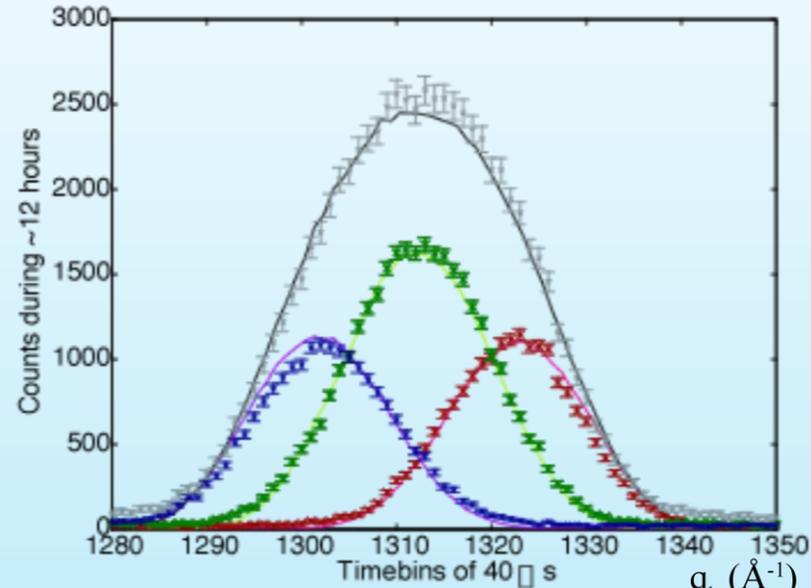
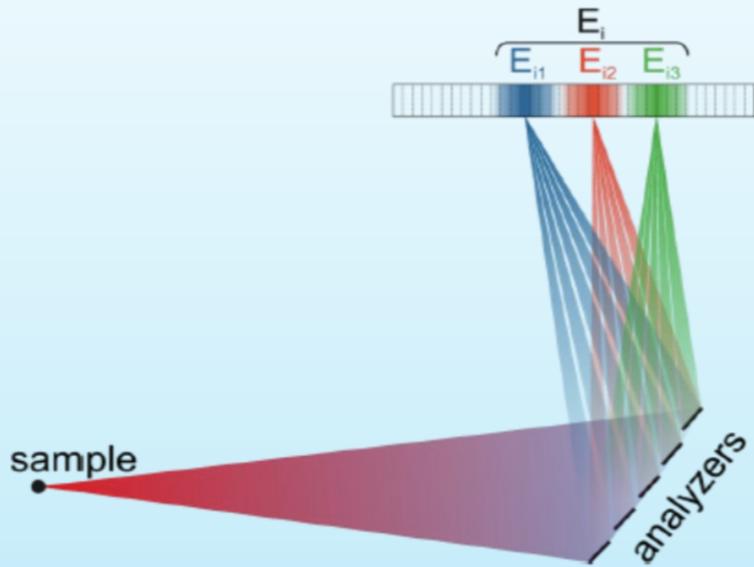
(evolved from CAMEA)

**BIFROST** – inverted geometry spectrometer

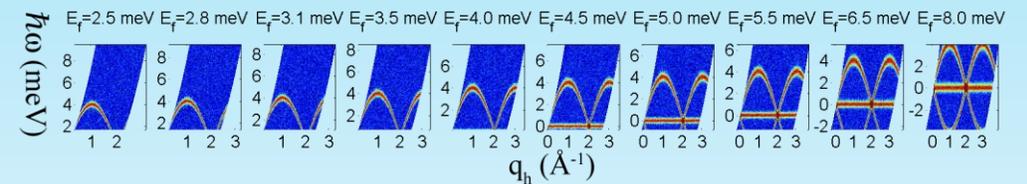


**BIFROST** primary spectrometer

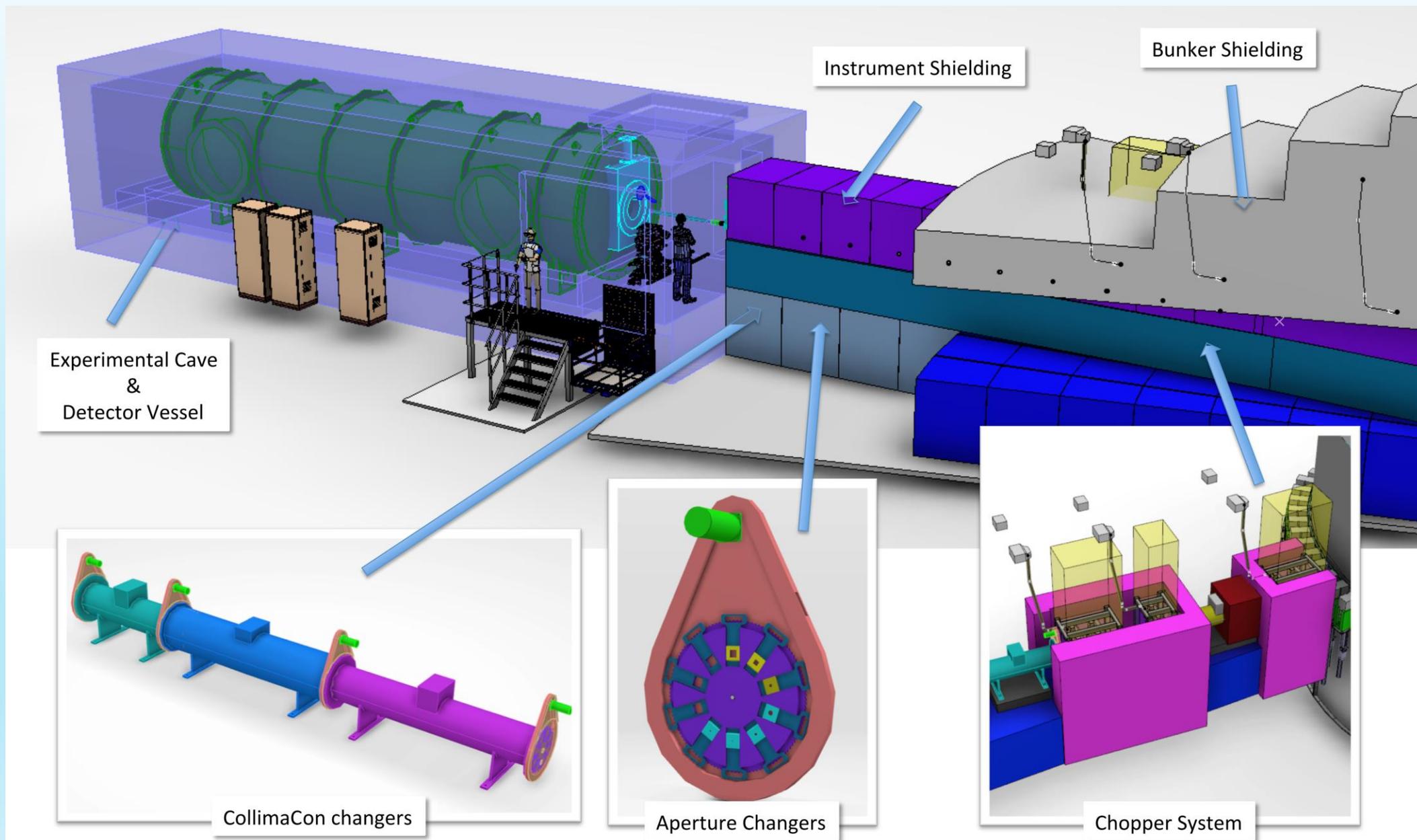
# BIFROST – Extreme Environment Spectrometer



**BIFROST** – the concept of prismatic spectroscopy

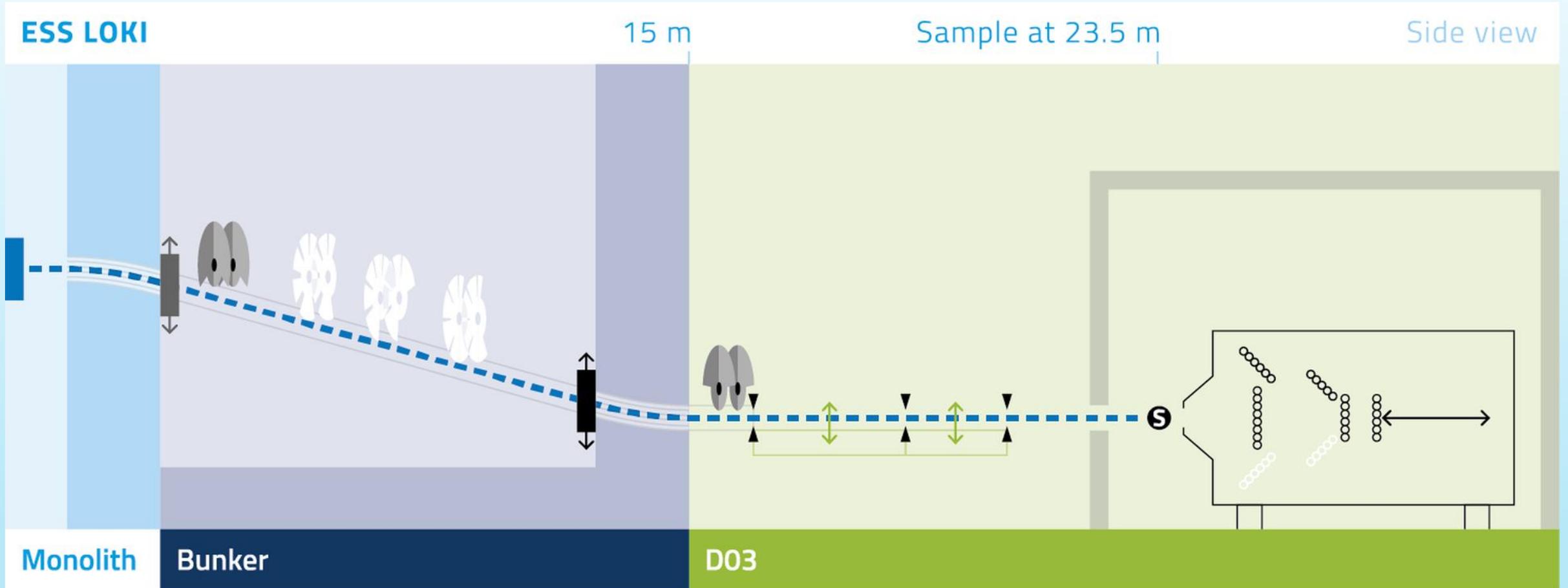


# LoKI – Broadband SANS



# LoKI – Broadband SANS

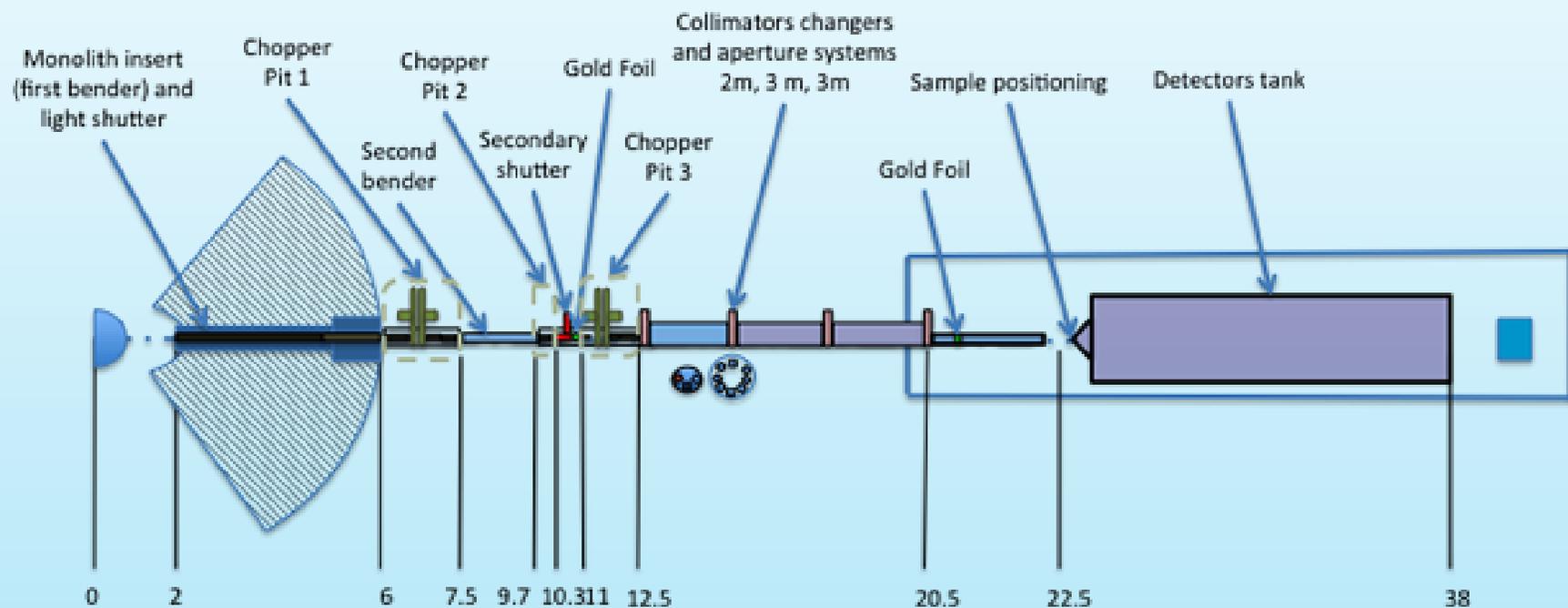
A broad Q range, high flux SANS instrument for soft matter, bio-science and materials science



LoKI is the shorter of the two SANS instruments being built at ESS. The sample position is located at 23.5 m from the source and the maximum sample-to-detector distance is 10 m.



# LoKI – Broadband SANS



**Loki**, the Norse god of mischief

(appears in Richard Wagner's opera cycle Ring of the Nibelung)

$$L1_{\max} = 10\text{m}$$

$$L2_{\max} = 10\text{m}$$

Repetition rate = 14Hz or 7Hz

$$\delta\lambda_{\max} = 10\text{\AA} \text{ at } 14\text{Hz}$$

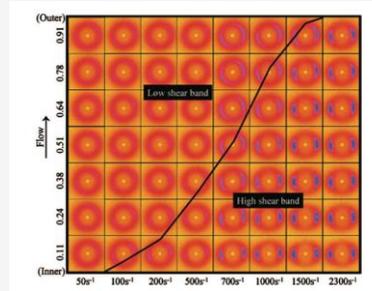
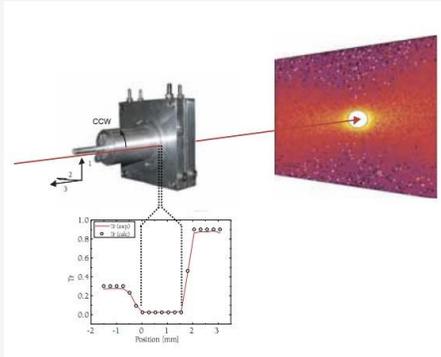
Max flux on sample  $\sim 1 \times 10^9 \text{ n/cm}^2/\text{s}$

2x line-of-sight closure

# LoKI – Broadband SANS

Shear Banding in CTAB wormlike micelles providing confirmation of rheological model. (Helgeson et al. (2009) J. Rheol 53, 727)

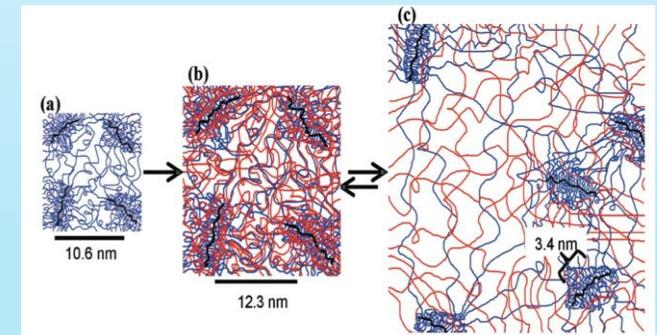
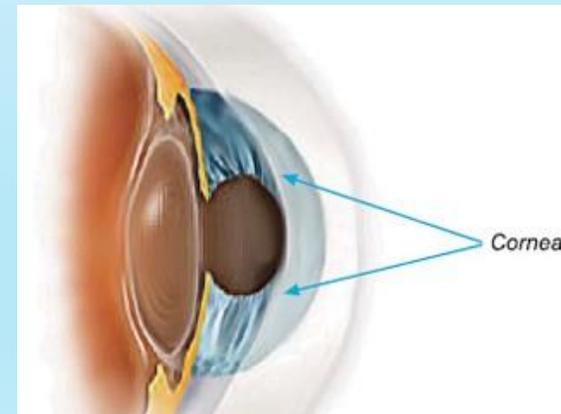
## FLOW



The flow of **complex fluids** through **complex geometries** is relevant to many industrial processes. There is a need to understand **structure effects of flow** both for practical purposes and to compare with fluid flow models.

## KINETICS

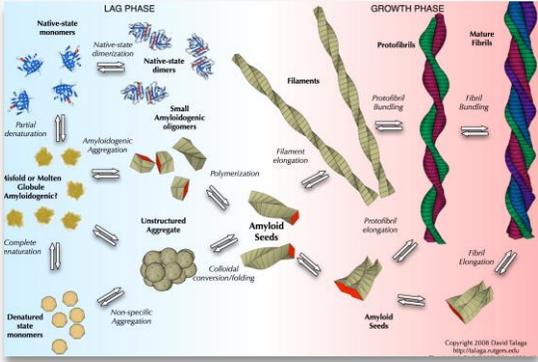
Gel structure forms over **multiple length scales**. Kinetics of gelation can be rapid needing **sub-second** time resolution. Neutrons provide the structure of each component in the presence of the other.



Swelling of a double network hydrogel designed for use as a cornea replacement. (Frank Group, Stanford)

# LoKI – Broadband SANS

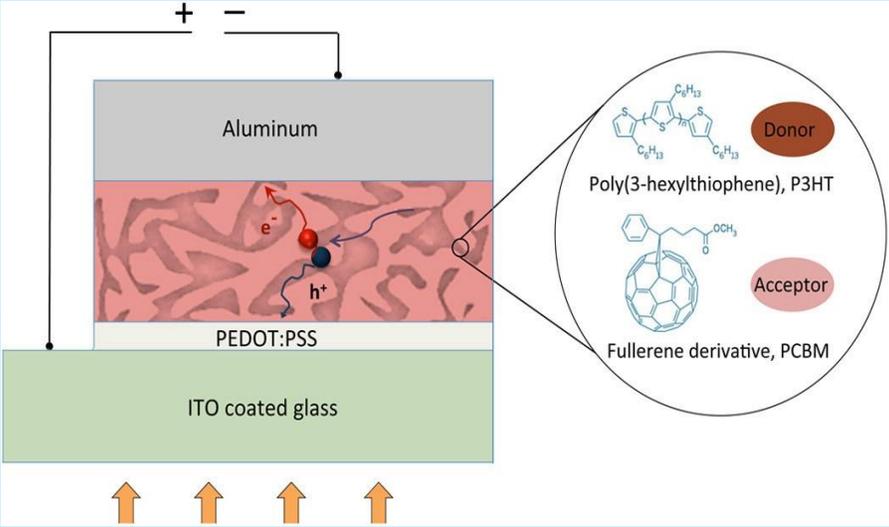
MULTI  
SCALE



Amyloid fibril formation and growth is a **multi-length scale problem** and to understand methods of formation and inhibition the structural evolution must be observed.

DEVICES

Organic Solar Cells promise to provide cheap and accessible solar energy. The **lifespan** and **efficiency** of the devices depends on the **nano-structure** polymer mixture. Understanding the **structural evolution** under operation guides development of new devices.



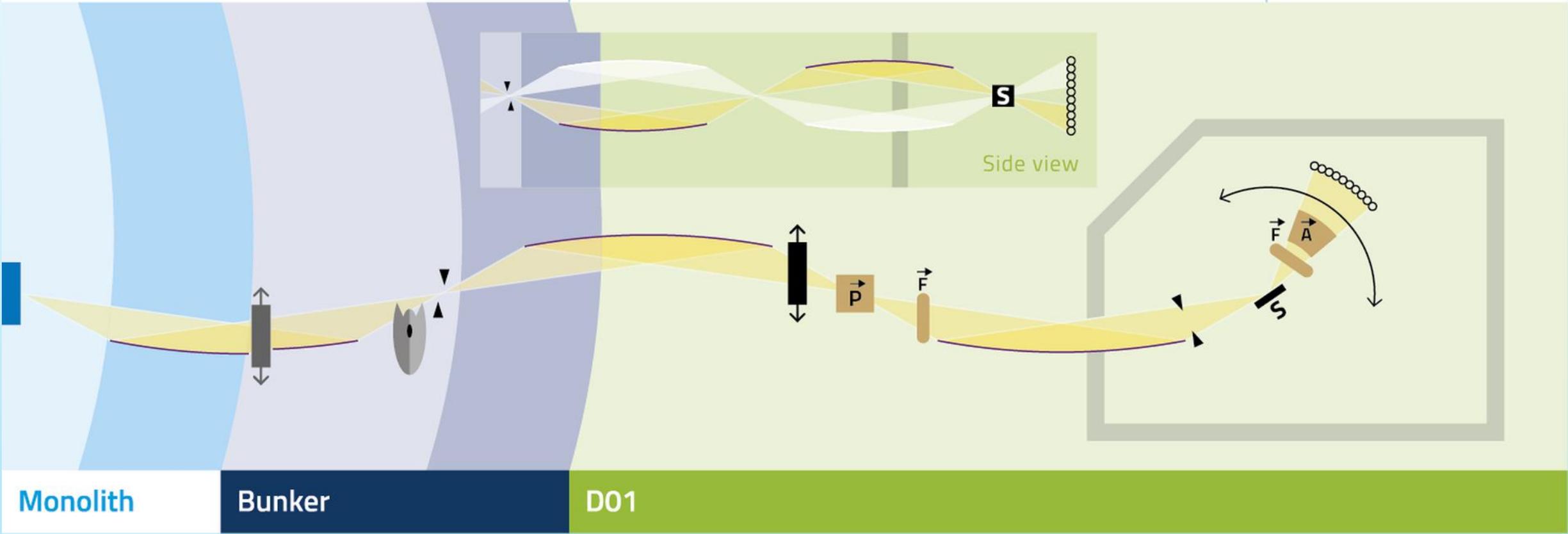
# ESTIA – Focusing Reflectometer

ESS ESTIA

15 m

Sample at 35 m

Top view



Monolith

Bunker

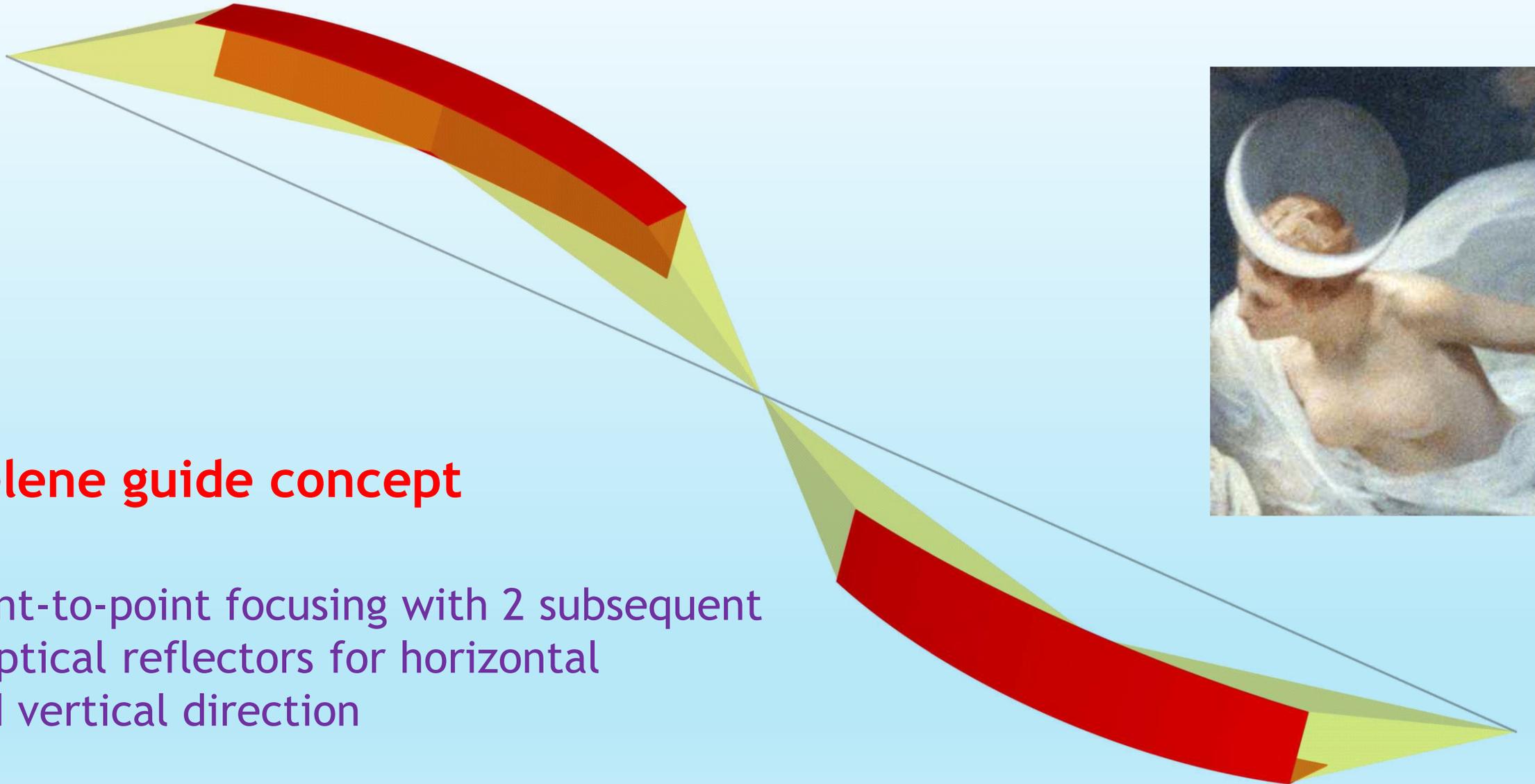
D01

# ESTIA – Selene guide concept

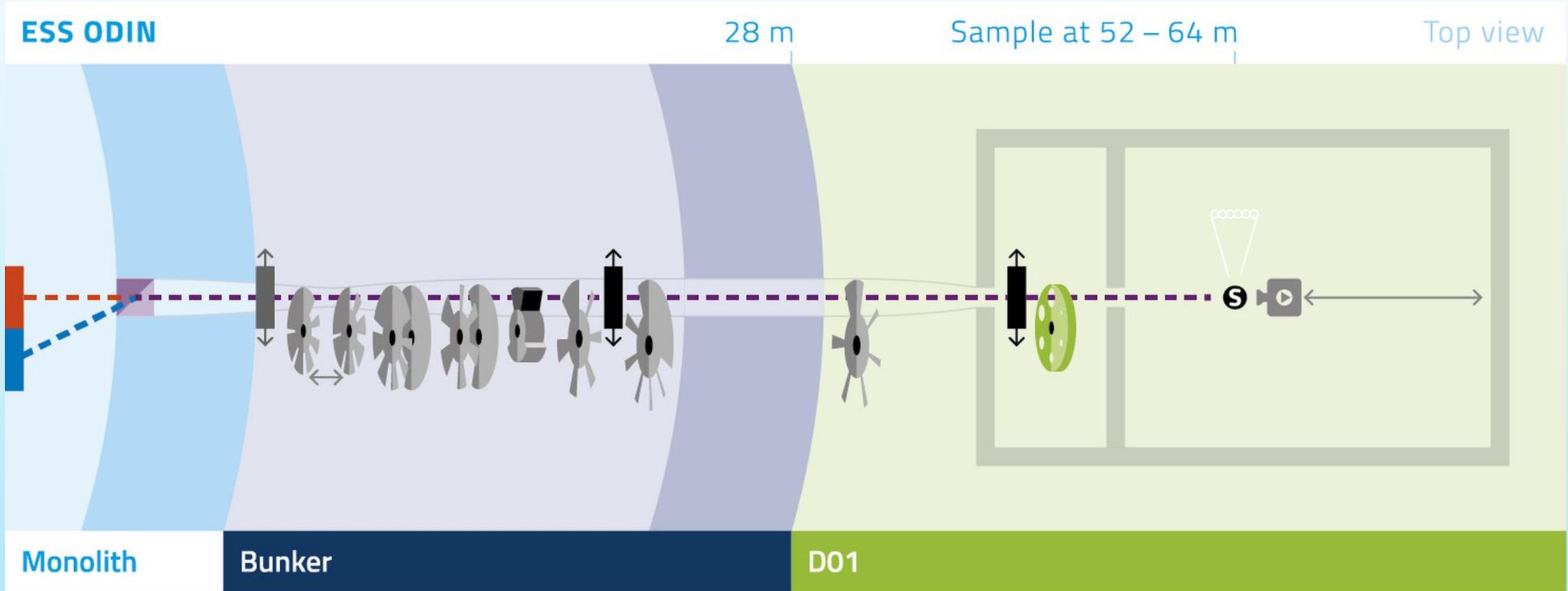


## Selene guide concept

point-to-point focusing with 2 subsequent elliptical reflectors for horizontal and vertical direction

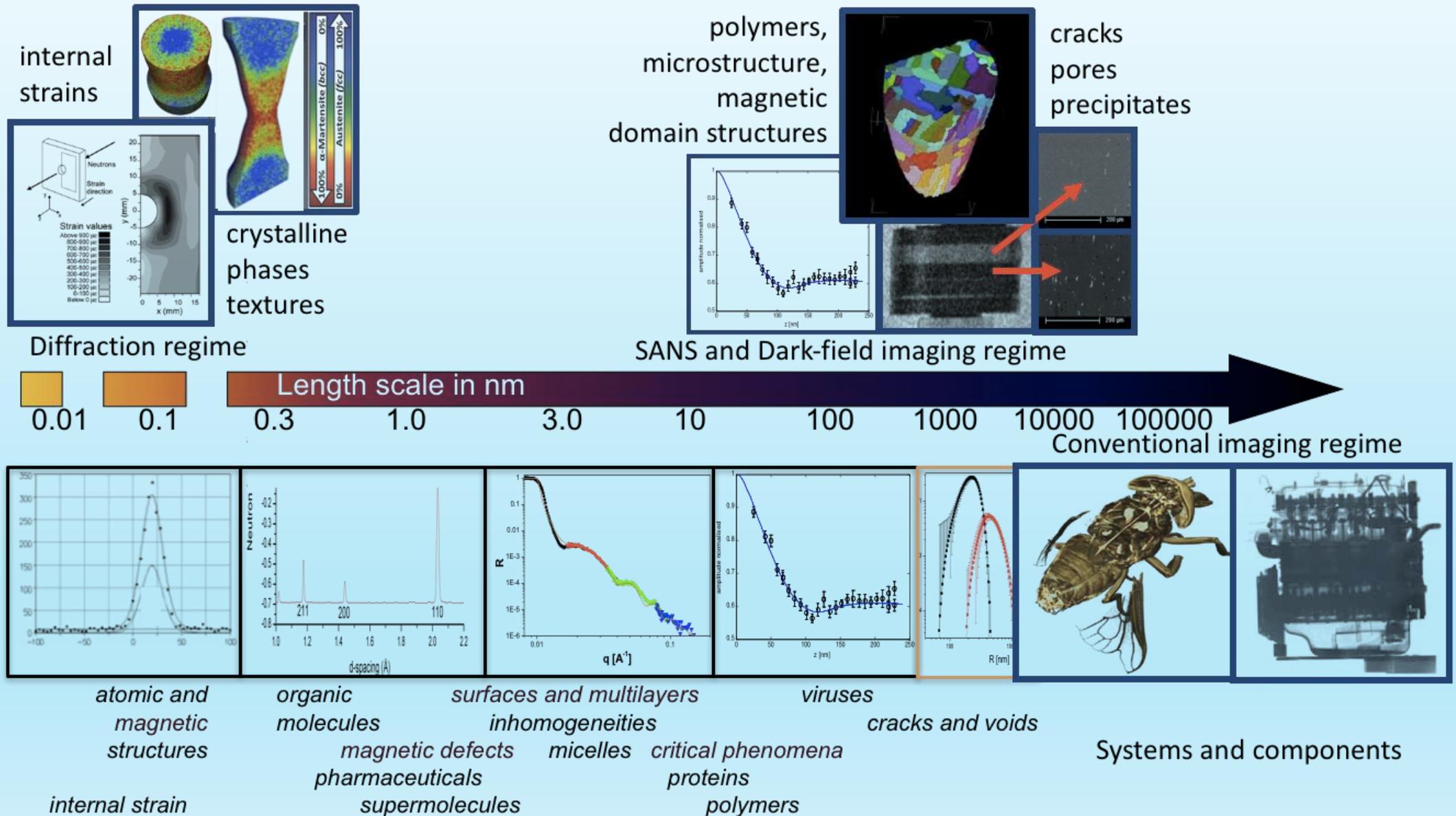


# ODIN – Multipurpose Imaging



**Neutron imaging** is a real-space technique examining the inner structure of potentially highly complex components and samples by detecting the transmitted beam.

# ODIN – Multipurpose Imaging



# Konsorcjum «Neutrony dla polskiej nauki» koordynowane przez



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