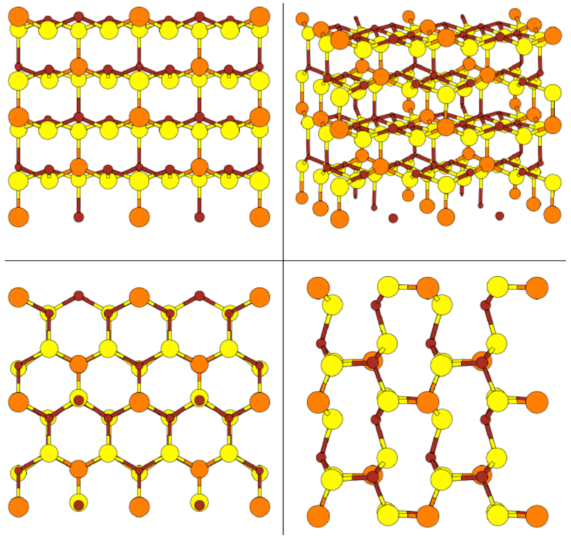
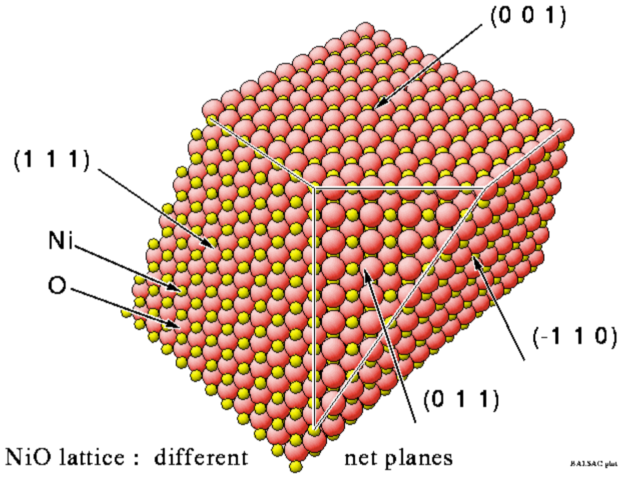
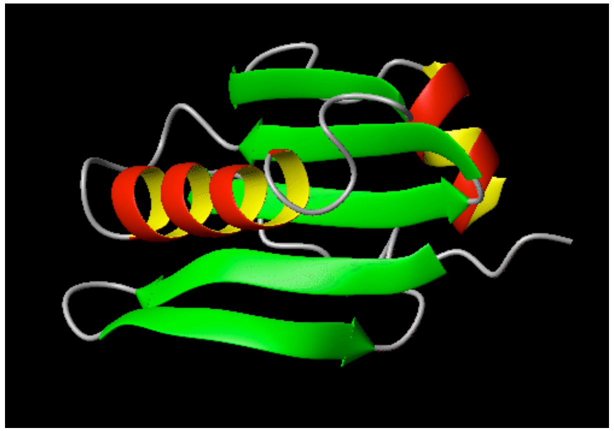
Opening-up the World of Materials

EPICS Summer School

Mission statement:
Opening-up the World of Materials
or Develop a GPS for atoms (and spins)







Determine both the structure and the fluctuations

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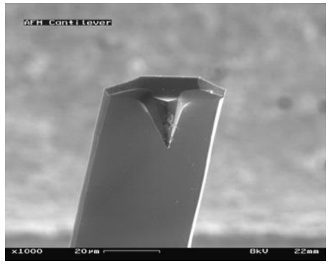
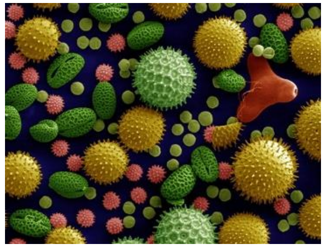
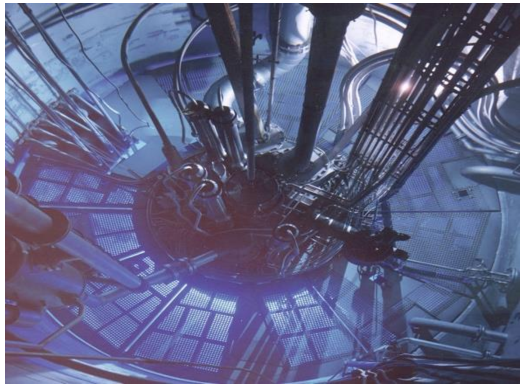





- Researchers have a vast toolbox at their disposition.
- When it comes to Large Scale Analytical Facilities Europe has the lead.
- Neutrons are an indispensable element of the box, and the ESS is Europe's next neutron flagship.

In addition to imaging, we use scattering.
The trick consists in converting distances into angles!
The wavelength acts as a conversion parameter.

energy

$$E = \frac{82}{\lambda^2} \quad [meV, Å]$$

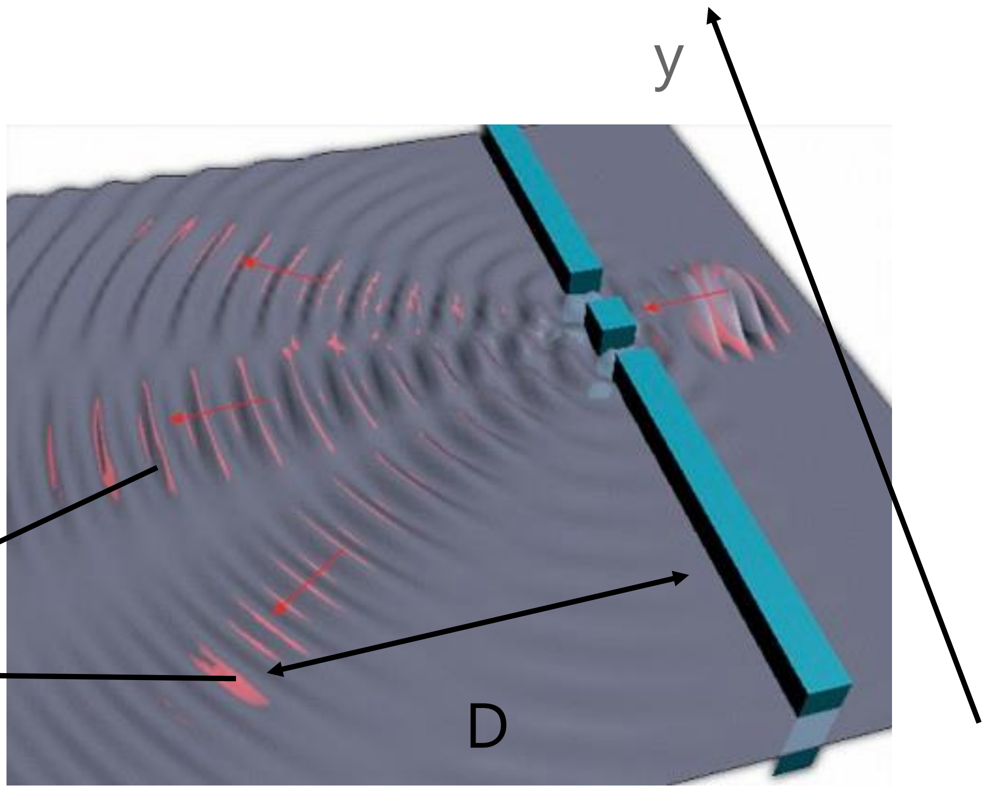
$$E \approx 2k^2 \quad [meV, Å^{-1}]$$

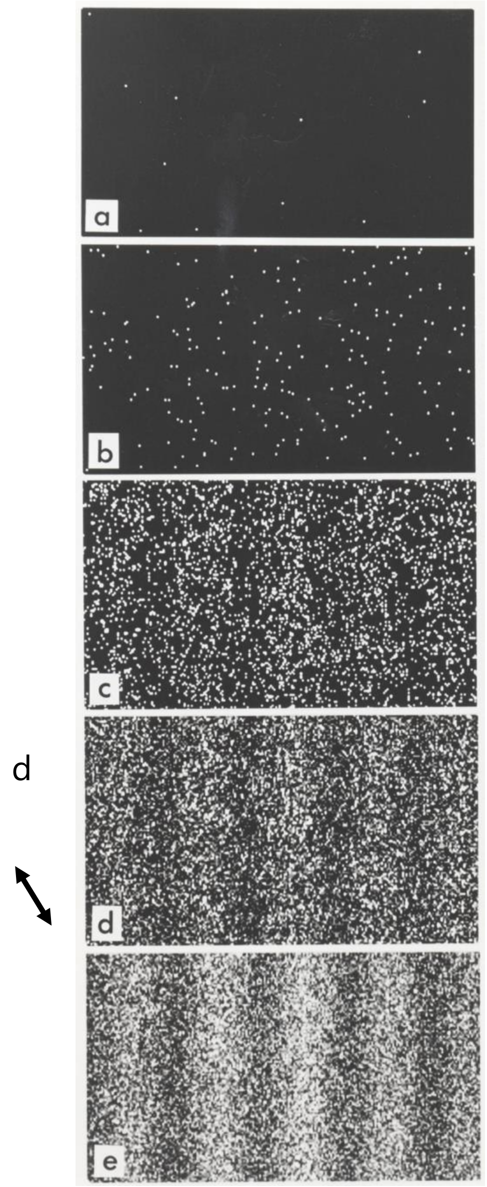
velocity

$$v = \frac{3960}{\lambda} \quad [m/s, Å]$$

$$I(y) \propto \cos^2\left(\pi \frac{d}{D}\frac{y}{\lambda}\right)$$

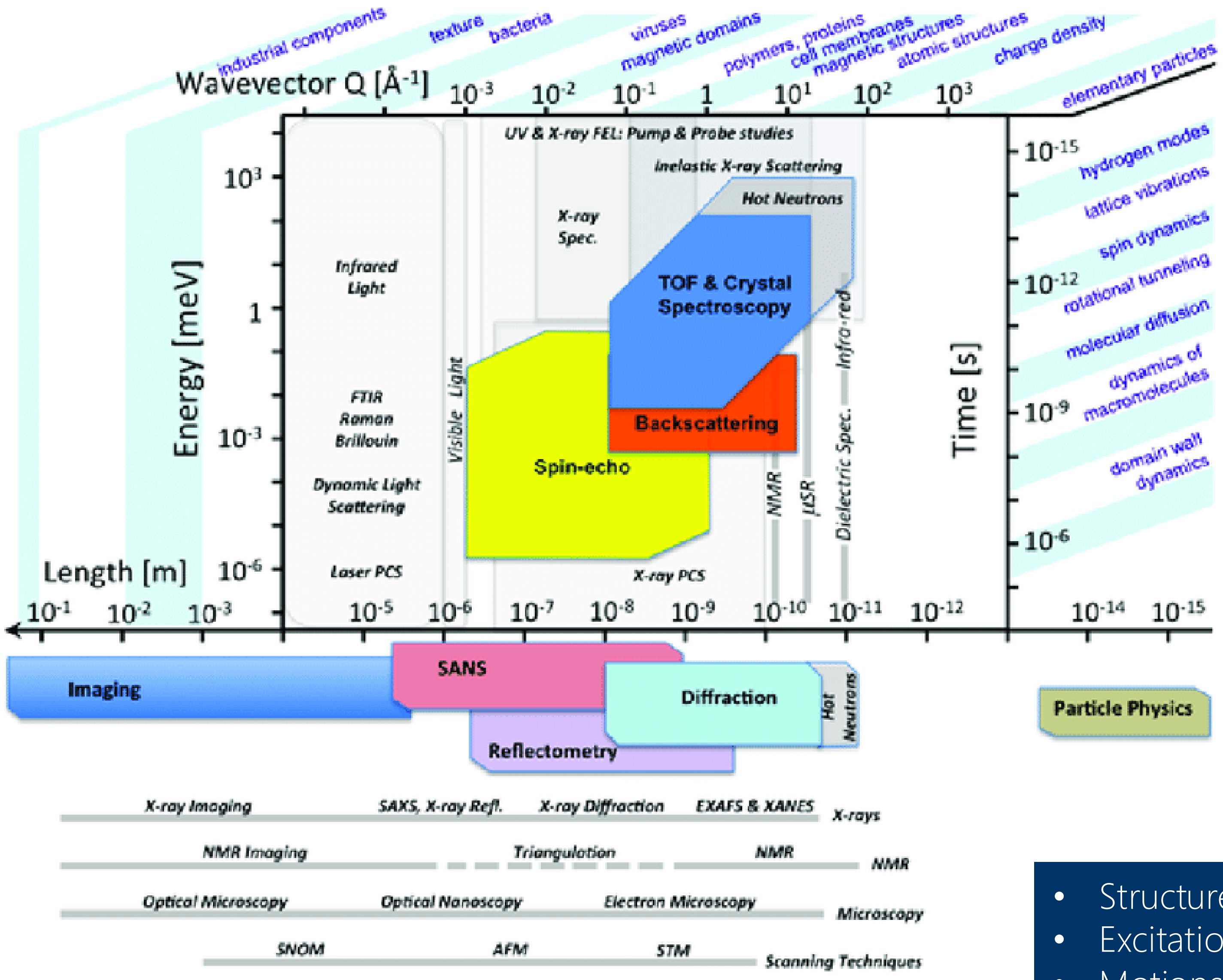
$$\Delta\phi = \frac{\Delta y}{D} = \frac{\lambda}{d}$$





Why neutrons matter!

- Access to the most relevant space and time dimensions.
- Direct and quantitative access to the relevant structural and dynamic information.
- Complementary contrast to X-rays.
- Extremely sensitive to magnetism.
- Possibility of contrast variation.
- Gentle probe, i.e., non-destructive.
- Highly penetrating.
- …



- Structure
- Excitations
- Motions and Relaxations

A few illustrative examples

Structure on the micro-scale: In-situ imaging

Monitoring CO_2 conversion

ACS Energy Letters
Open Access
http://pubs.acs.org/journal/aelccp

High-Resolution Neutron Imaging of Water Transport in CO_2 Electrolysis during Pulsed Operation

Luca Bohn, Josephine Häberlein, Frederik Brendel, Lukas Metzler, Lukas Helfen, Alessandro Tengattini, Carolin Klose, Severin Vierrath, and Joey Disch*

Cite This: ACS Energy Lett. 2025, 10, 975−981 Read Online

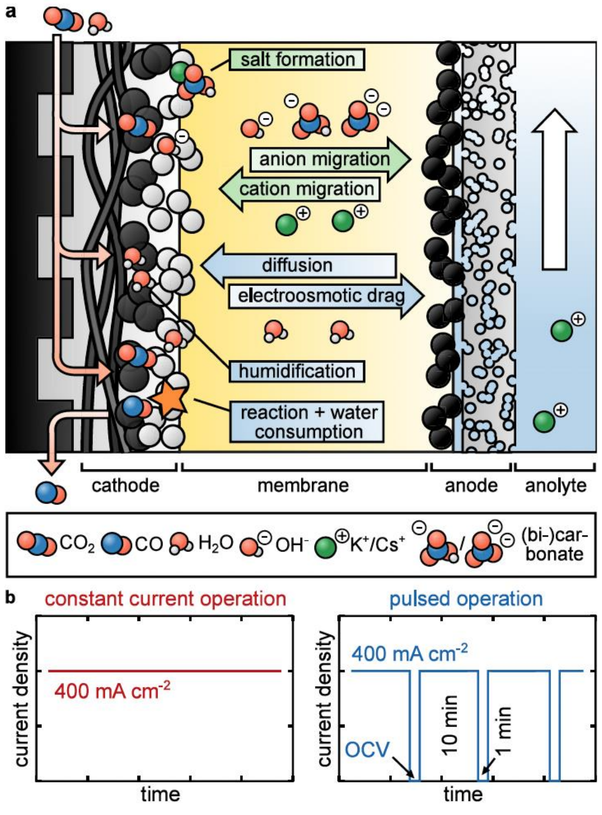
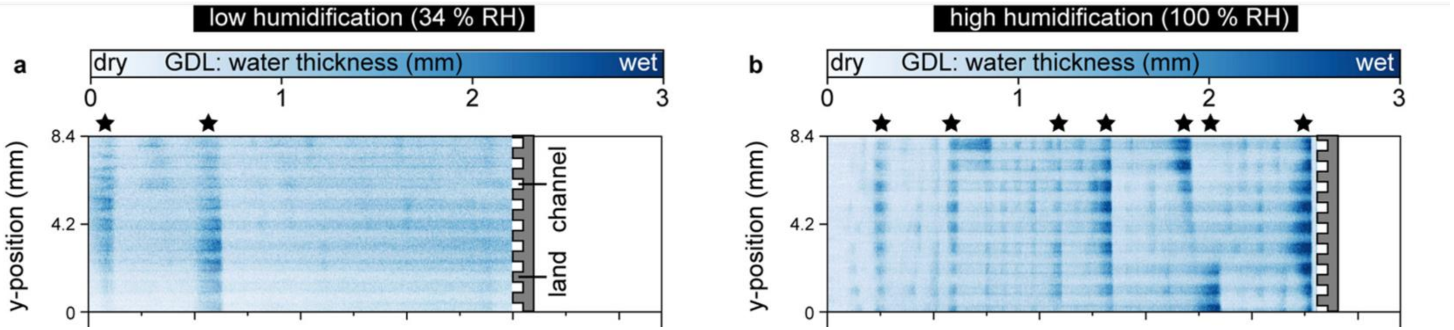
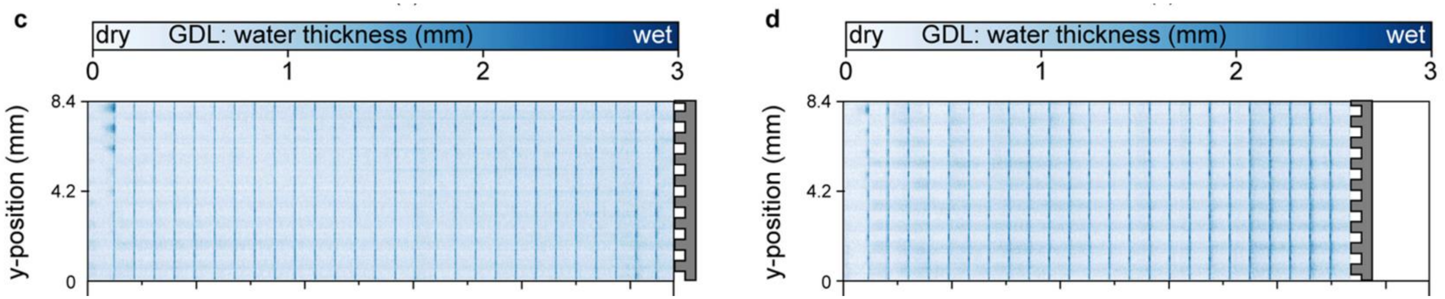


Figure 1. Transport processes and operation mode. a) Ion (green) and water (blue) transport processes in an alkaline zero-gap CO_2 electrolyzer. b) Constant current and pulsed operation mode.

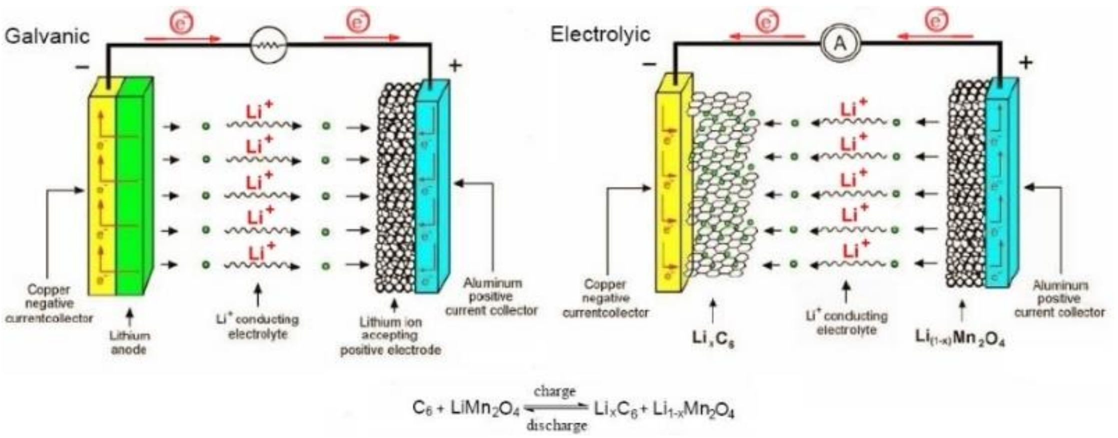
Continuous current operation

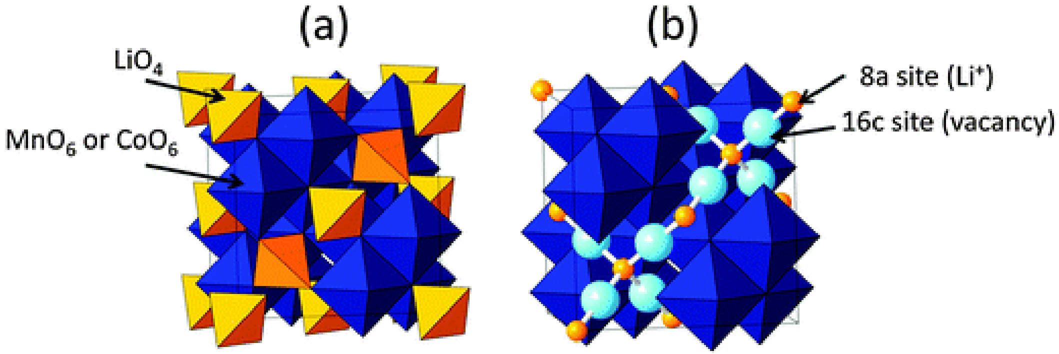


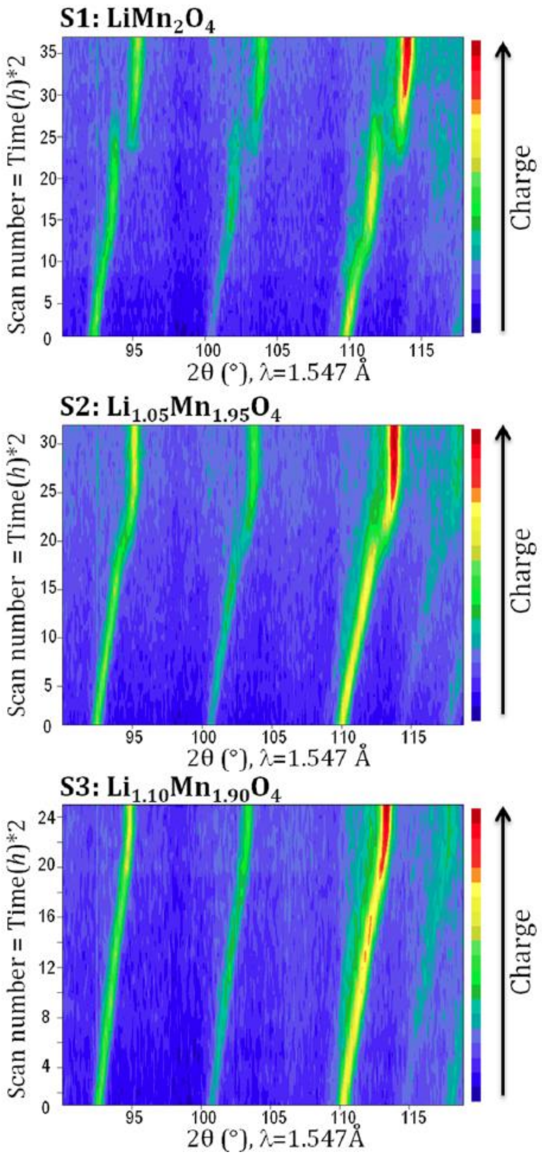
Pulsed current operation



Observing batteries in operando



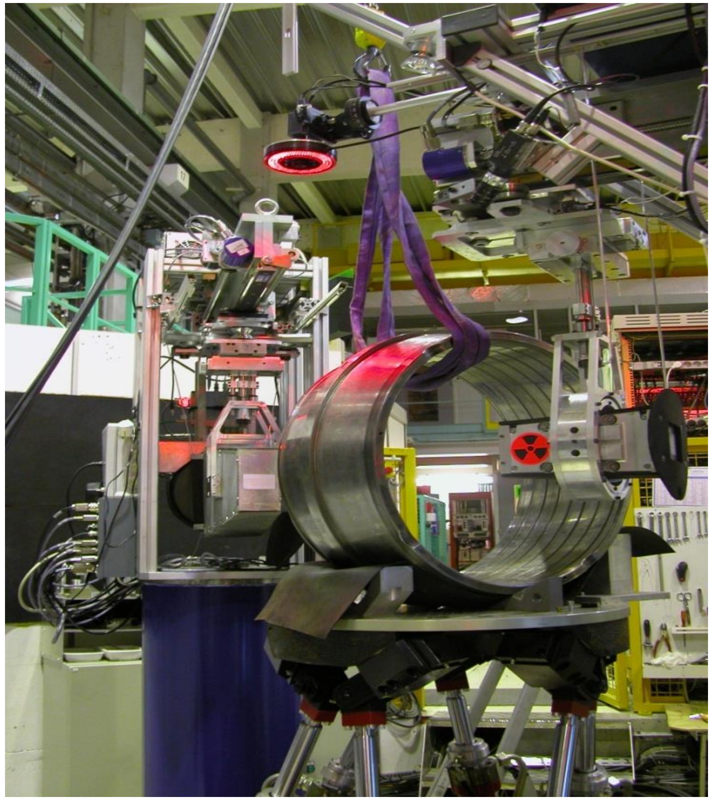


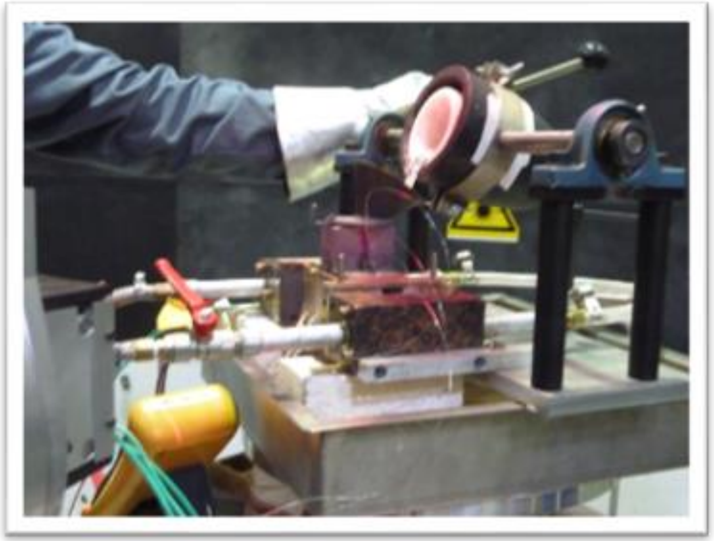


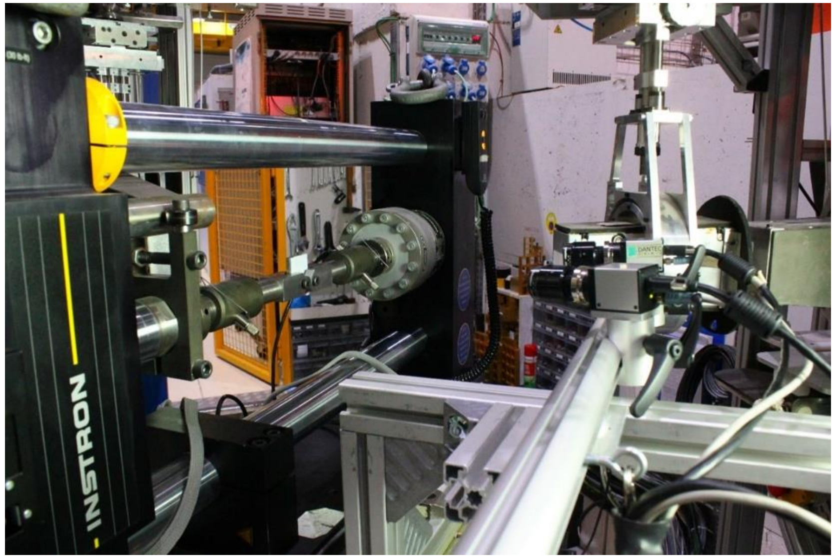
Matteo Bianchini, Emmanuelle Suard, Laurence Croguennec, and Christian Masquelier, Journal of Physical Chemistry C, 2014.

Strain scanning

Reduce device failure, improve production processes, and quality control



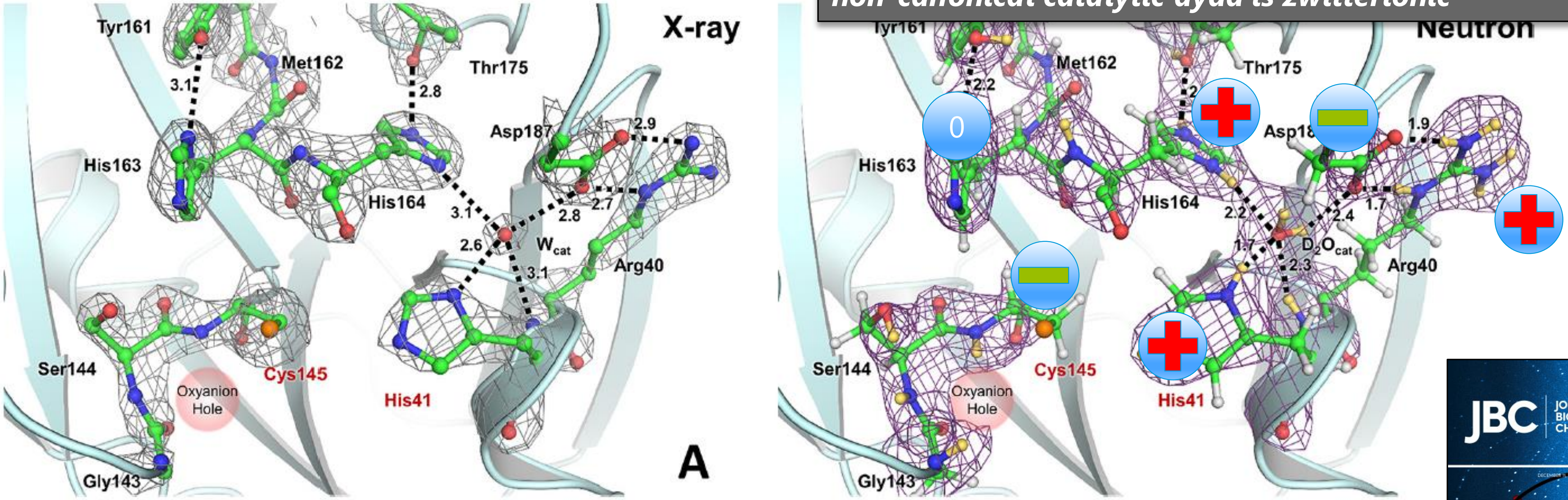


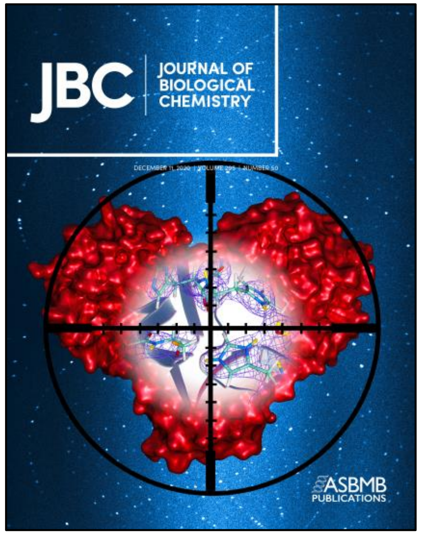


Courtesy: ILL

Helping fight diseases
Understanding the main Protease of Sars-CoV-2

First cysteine (coronavirus) protease neutron structure:
non-canonical catalytic dyad is zwitterionic

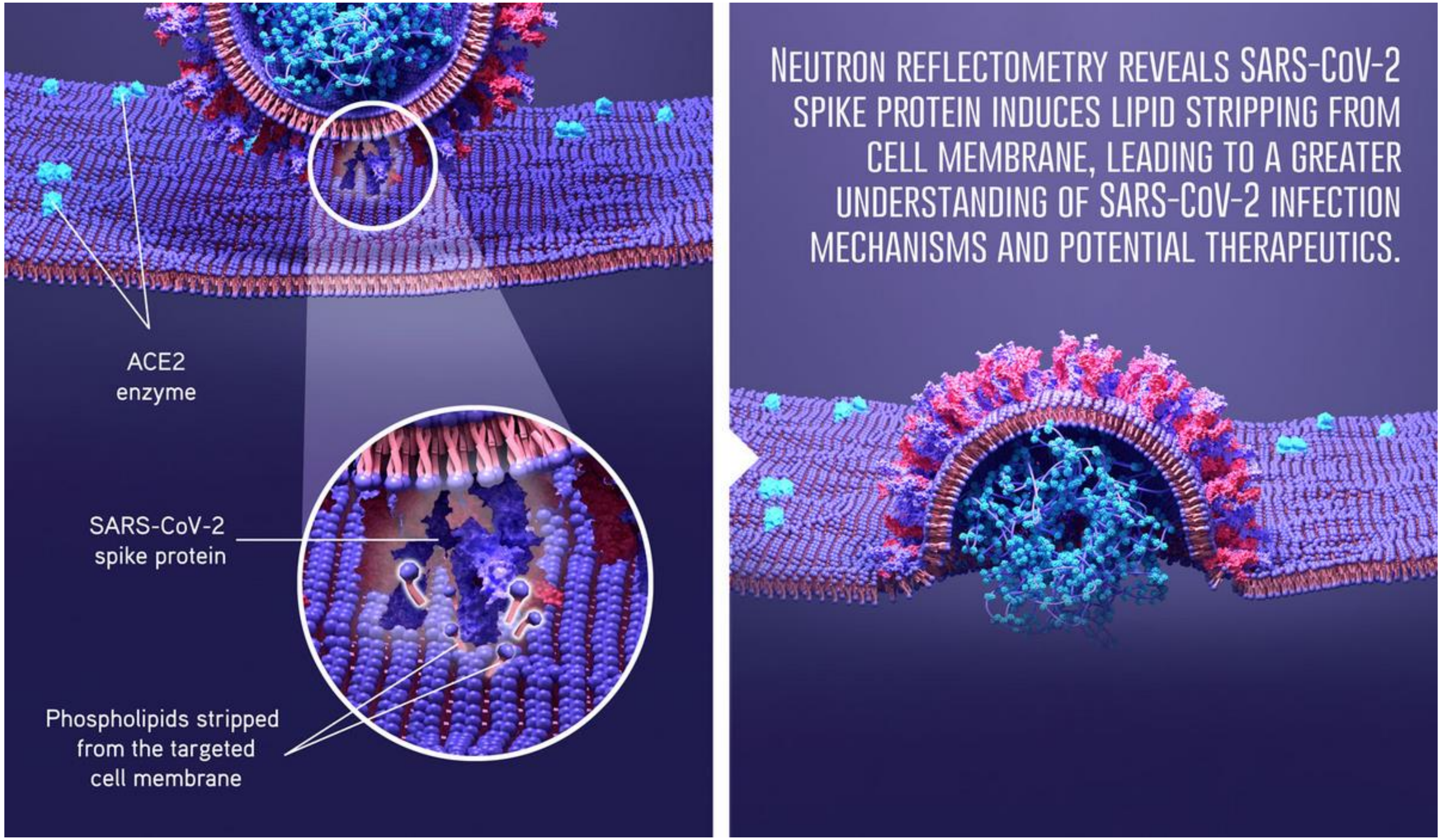




To understand the enzymatic process it is important to know the charge state.
With more than 100 chemical choices at hand experimental insight is needed.
This insight can today only be provided by neutron diffraction.

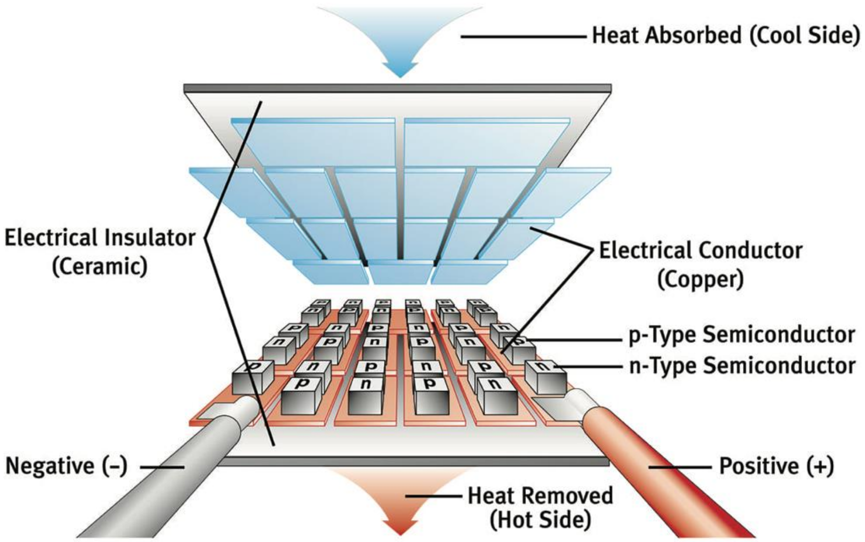
Kneller et al. *J. Biol. Chem.* 2020

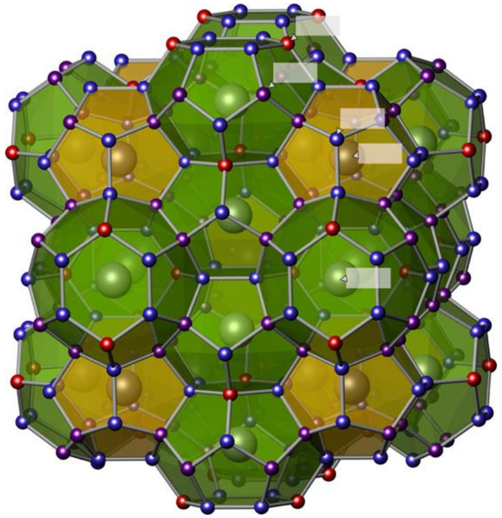
Helping fight diseases
Exploring non-canonical interactions

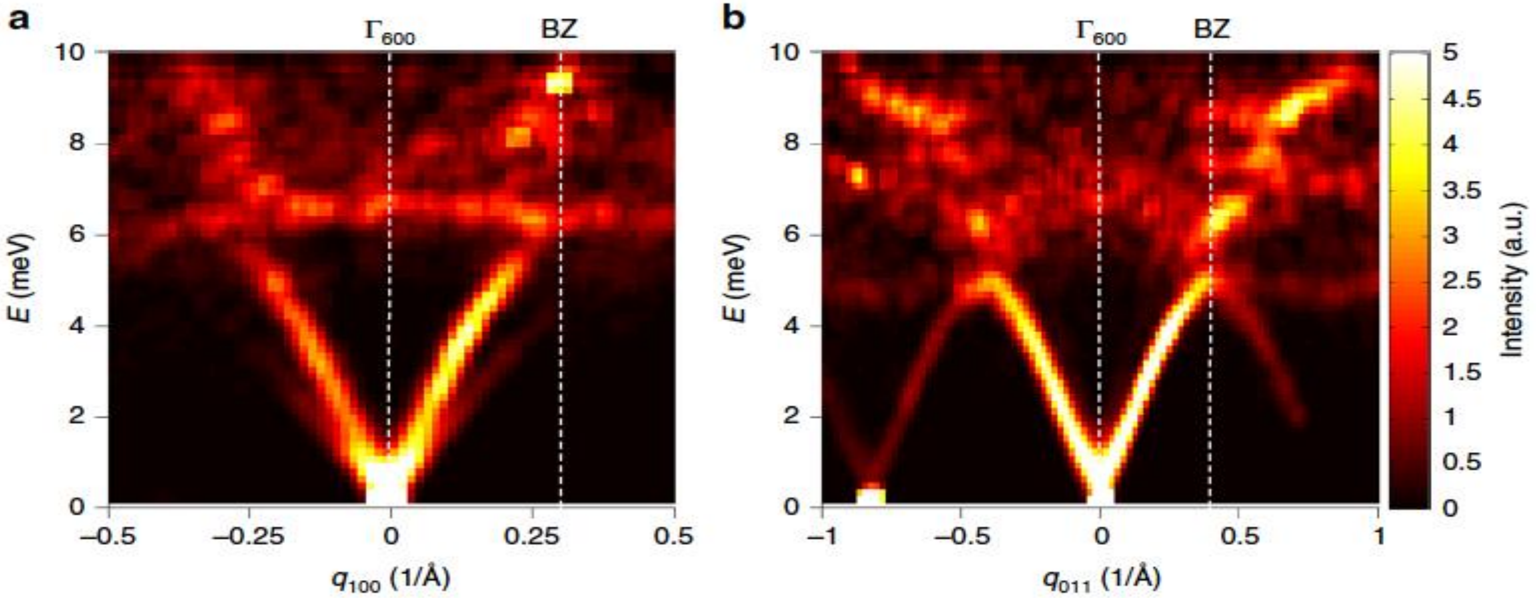


Alessandra Luchini et al., Scientific Report, 2021

Determining thermal conductivity








nature COMMUNICATIONS

ARTICLE

DOI: 10.1038/s41467-017-00584-7 OPEN

Direct measurement of individual phonon lifetimes in the clathrate compound $Ba_{7.81}Ge_{40.67}Au_{5.33}$

Pierre-François Lory[1,2], Stéphane Pailhès[3], Valentina M. Giordano[3], Holger Euchner[4], Hong Duong Nguyen[5], Reiner Ramlau[5], Horst Borrmann[5], Marcus Schmidt[5], Michael Baitinger[5], Matthias Ikeda[6], Petr Tomeš[6], Marek Mihalkovič[7], Céline Allio[8], Mark Robert Johnson[1], Helmut Schober[1,9], Yvan Sidis[10], Frédéric Bourdarot[11], Louis Pierre Regnault[11], Jacques Ollivier[1], Silke Paschen[6], Yuri Grin[5] & Marc de Boissieu[2]

Quantum topology

Measuring entanglement

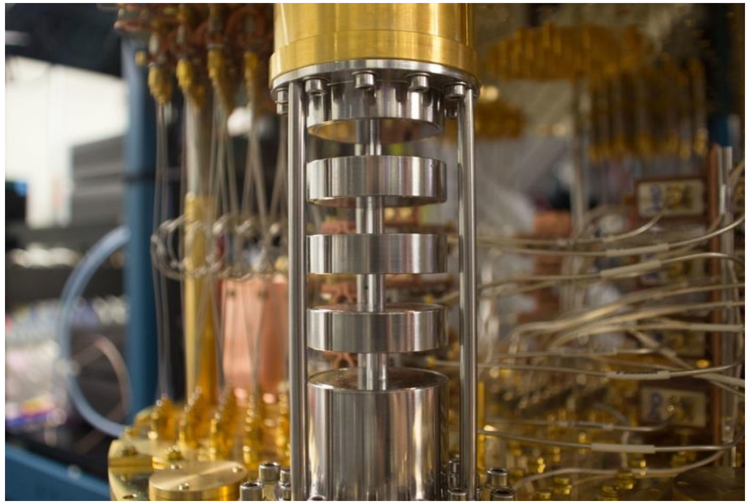
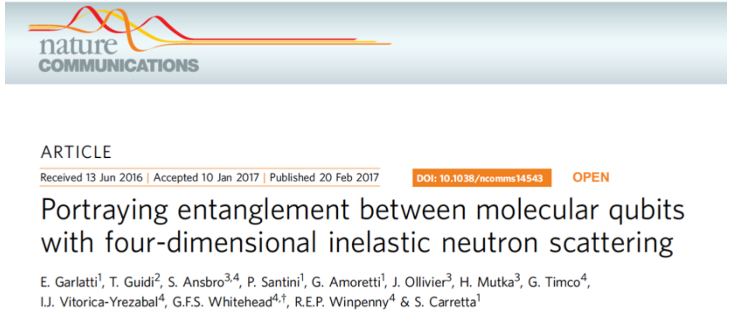


Image credit - Flickr/ IBM Research, licensed under CC BY-ND 2.0


nature COMMUNICATIONS

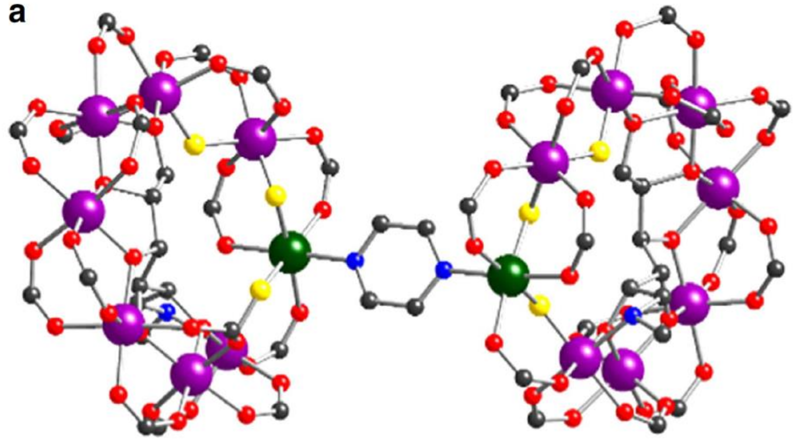
ARTICLE

Received 13 Jun 2016 | Accepted 10 Jan 2017 | Published 20 Feb 2017 DOI: 10.1038/ncomms14543 OPEN

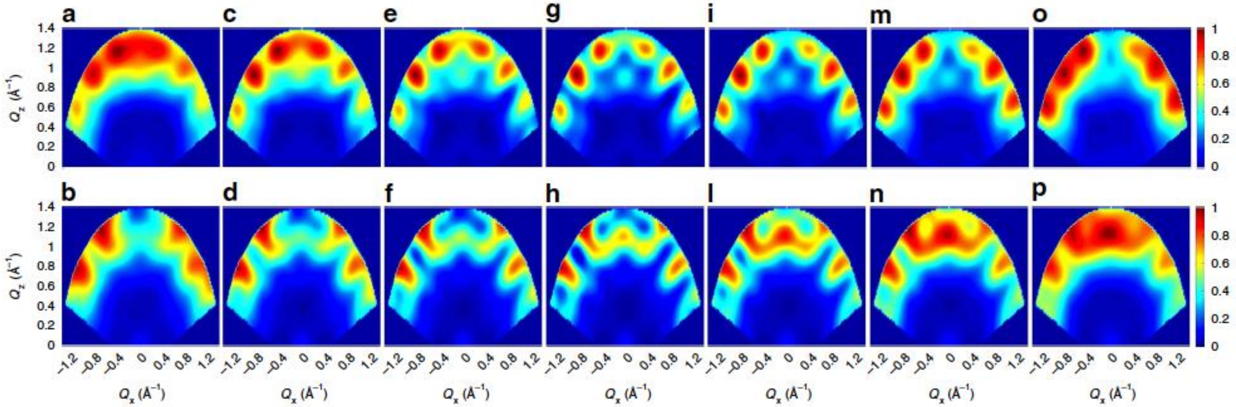
Portraying entanglement between molecular qubits with four-dimensional inelastic neutron scattering

E. Garlatti[1], T. Guidi[2], S. Ansbro[3,4], P. Santini[1], G. Amoretti[1], J. Ollivier[3], H. Mutka[3], G. Timco[4], I.J. Vitorica-Yrezabal[4], G.F.S. Whitehead[4,†], R.E.P. Winpenny[4] & S. Carretta[1]

$(Cr_7Ni)_2$ supra-molecular dimer



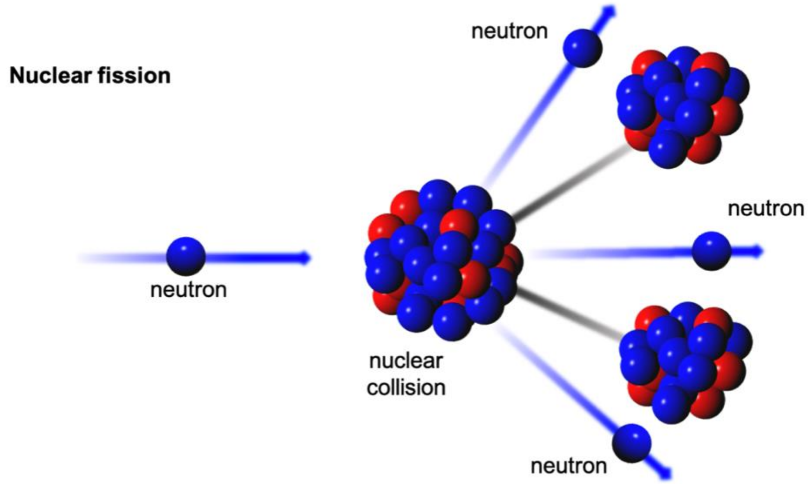
Two weakly coupled quantum bits (S=1/2)

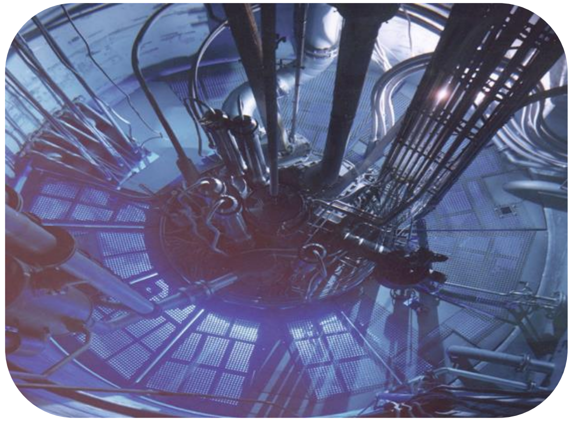


How do we create intense beams of neutrons!

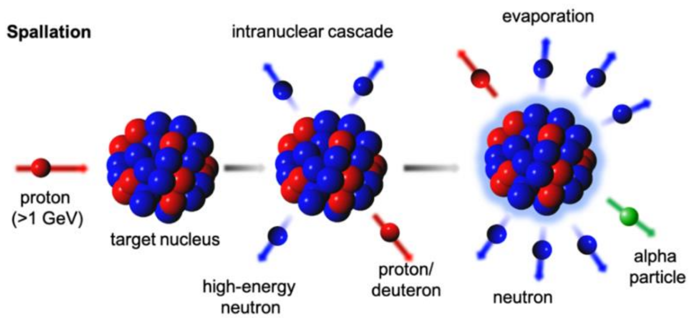
Freeing the neutrons from the nucleus

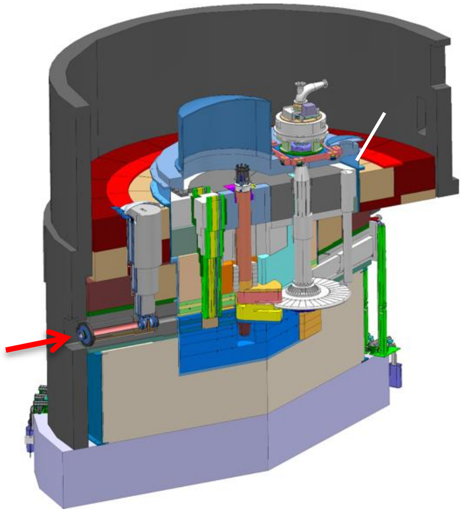
Fission



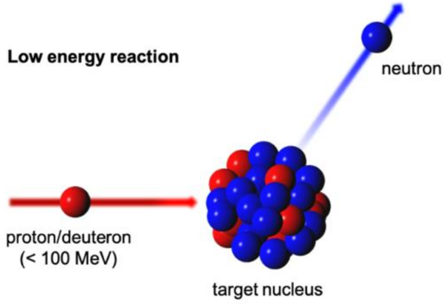


Spallation





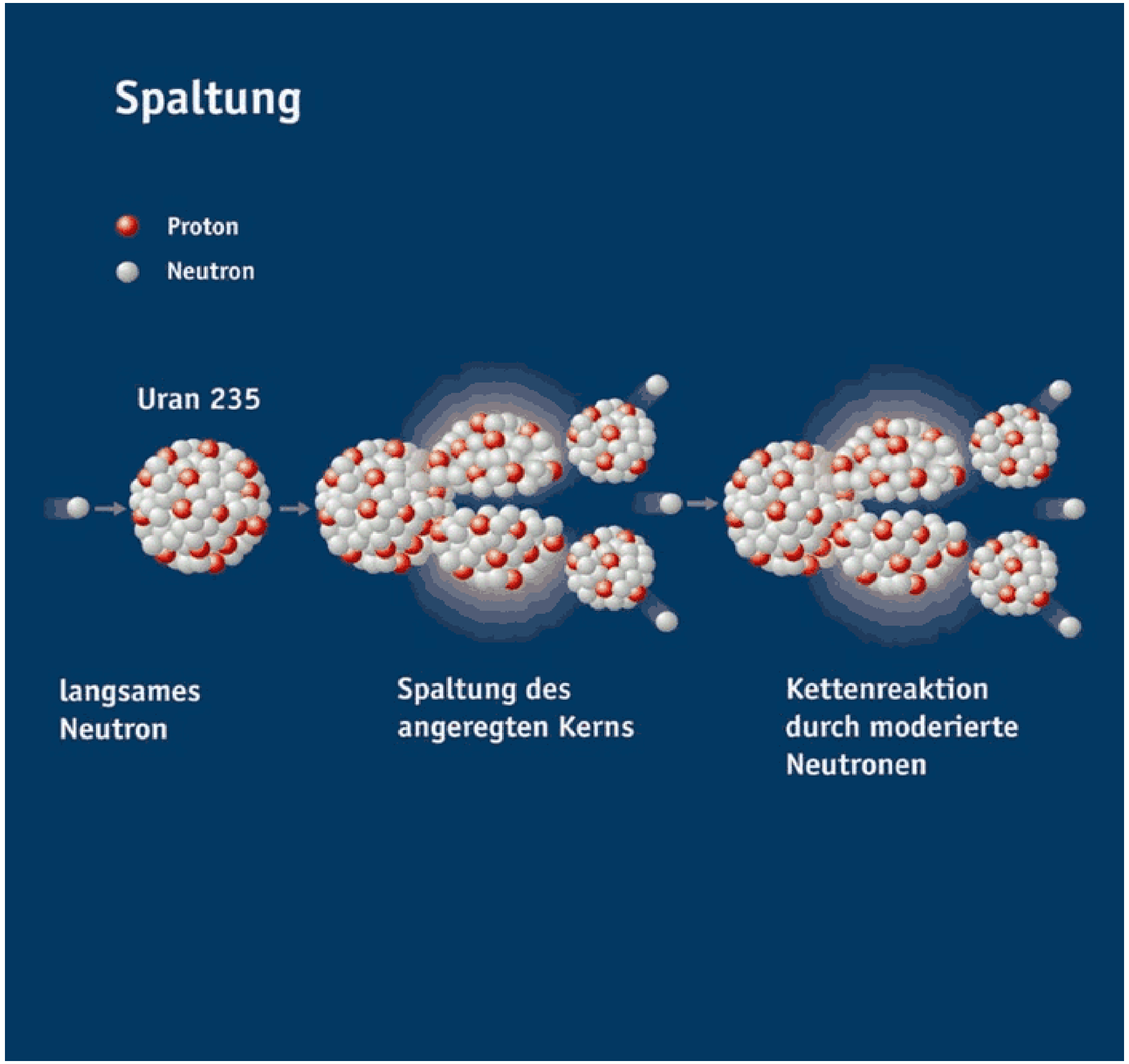
HiCANS



Spallation offers
- highest efficiency
- no criticallity
- pulsed operation

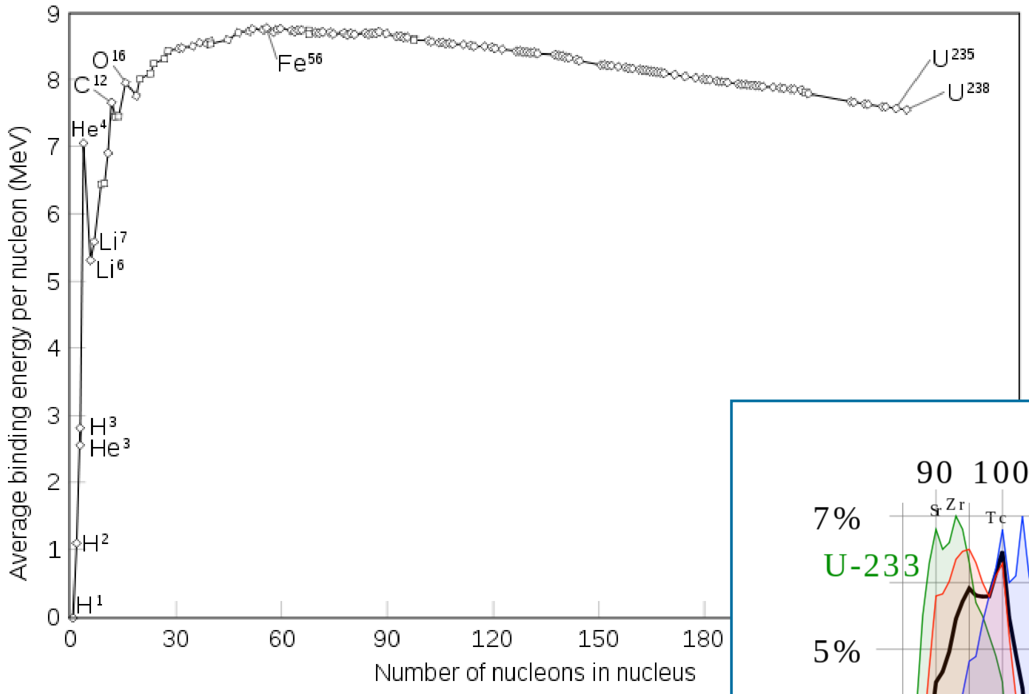
It requires sophisticated
- powerful accelerators
- resilient targets

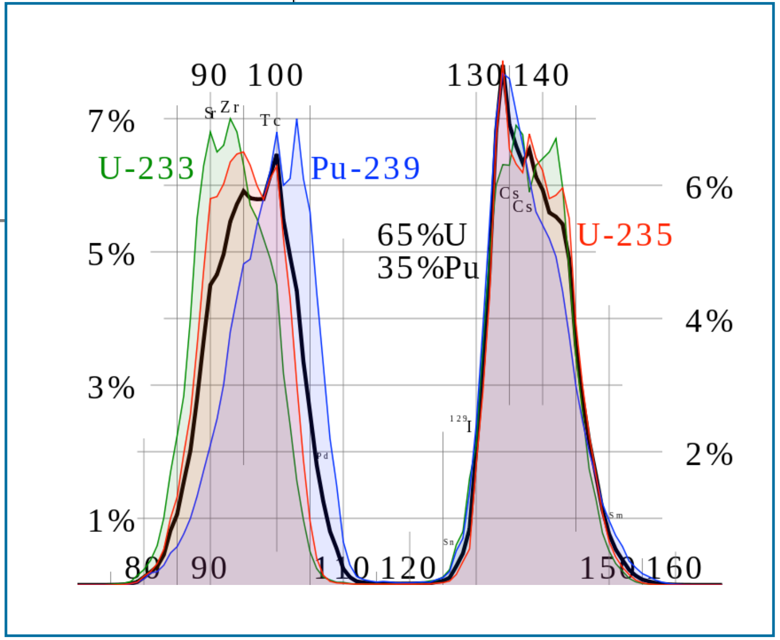
Fission in a reactor



Getting the neutrons out of the nucleus

Fission Basics





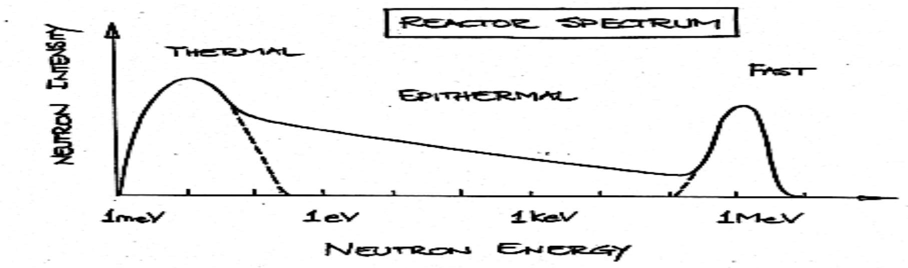
- Each fission event yields about 202.5 MeV of energy
  - ★181 MeV prompt fission energy
    - 169 MeV kinetic energy of daughter nuclei
    - 4.8 MeV for 2.5 neutrons
    - ≈7 MeV prompt gamma rays
  - ★21 MeV delayed fission energy
    - β-decay of fission products that are too rich in neutrons to be stable

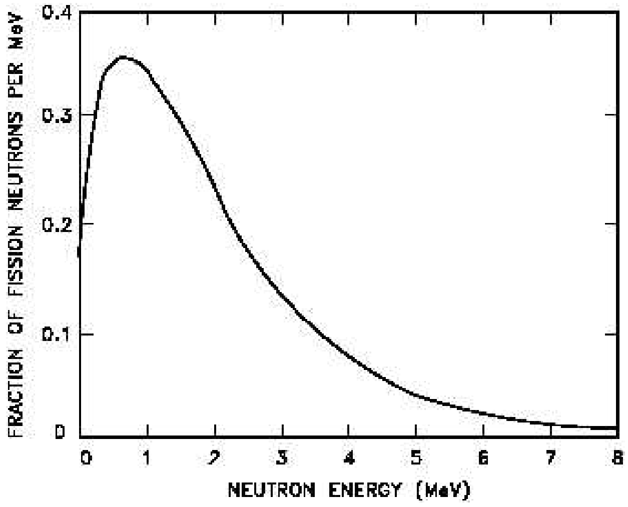
Getting the neutrons out of the nucleus

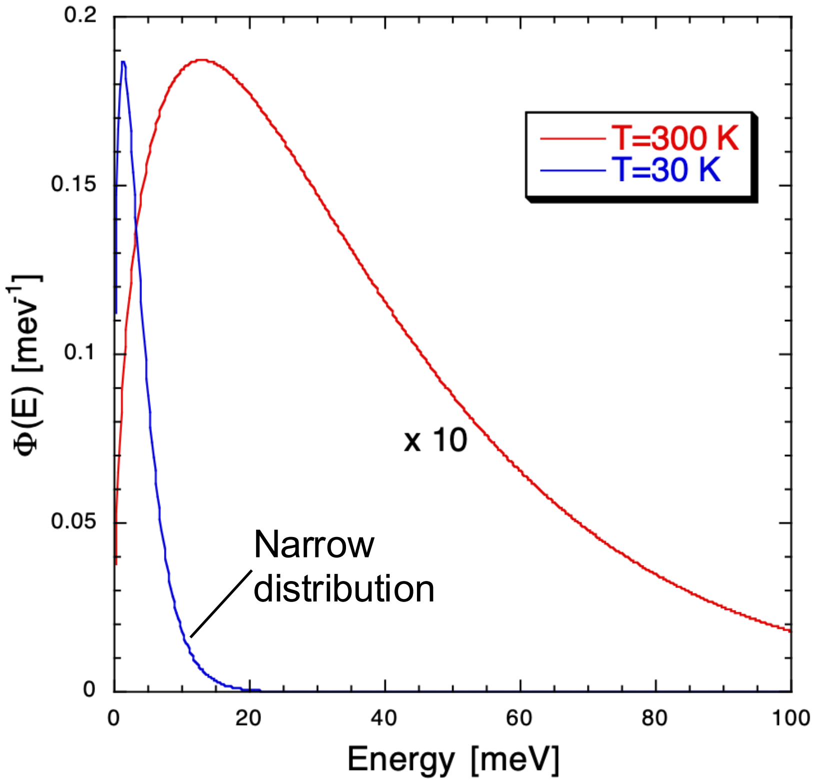
Fission Basics

The reactor neutrons are too energetic for most of our purposes (irradiation is an exception).

We must moderate them.



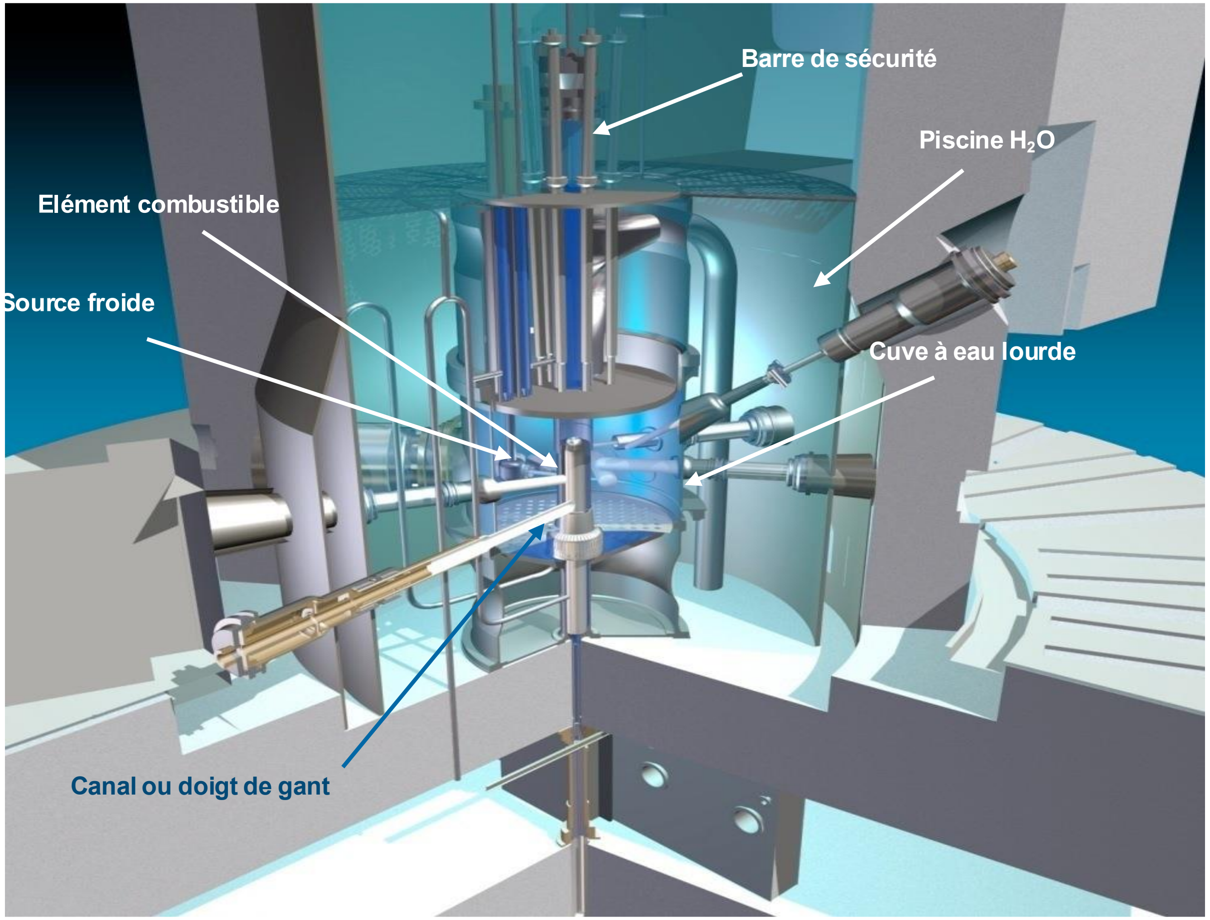




Cold Neutrons	0.1-10 meV
Thermal Neutrons	10-100 meV
Hot Neutrons	100 - 500 meV
Epithermal Neutrons	> 500 meV

The reactor core

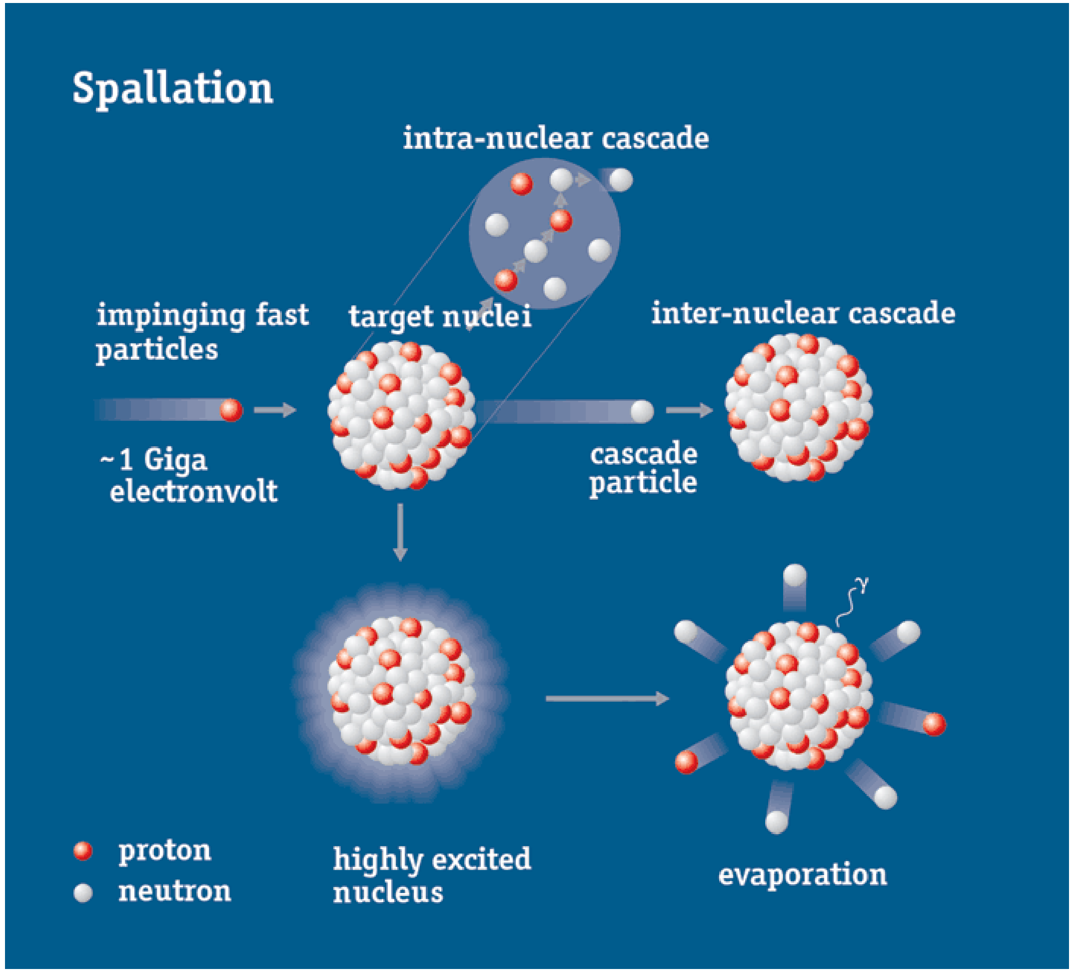
As compact as possible

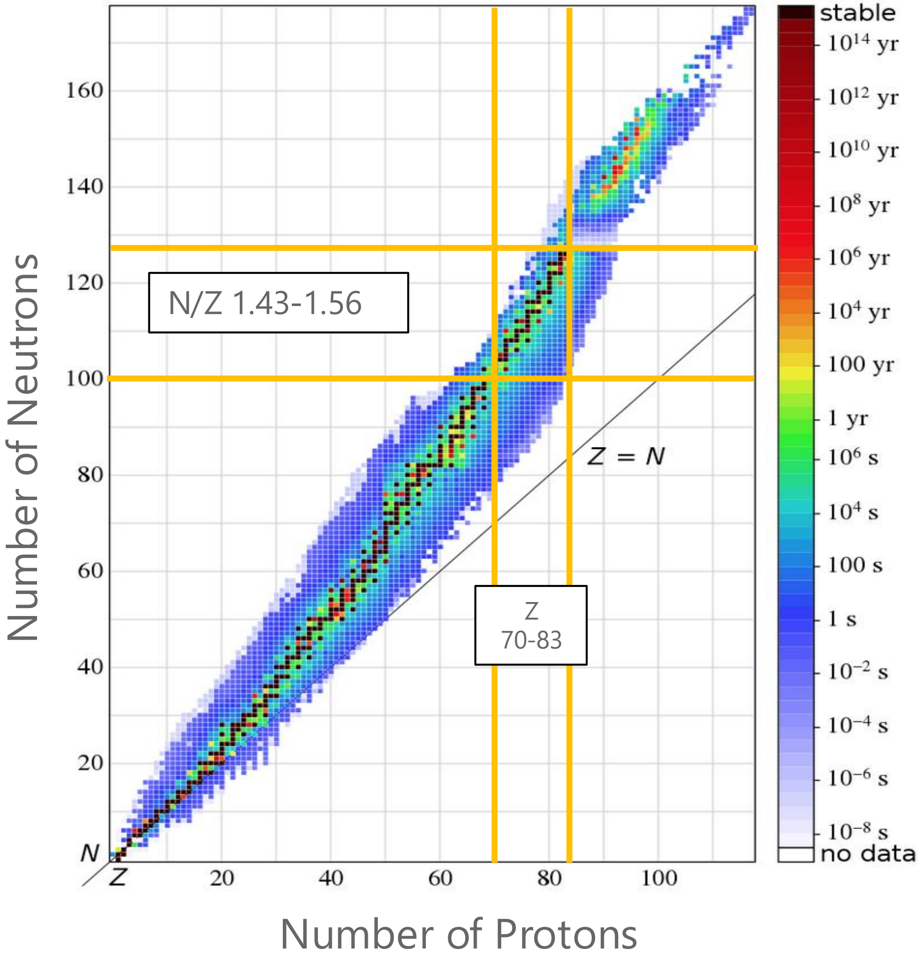


Moderation via D_2O, delayed neutrons from the moderator are essential for the control
UAl fuel element (currently still 93 % HEU), as compact as possible.

Courtesy: ILL

Spallation using a proton accelerator

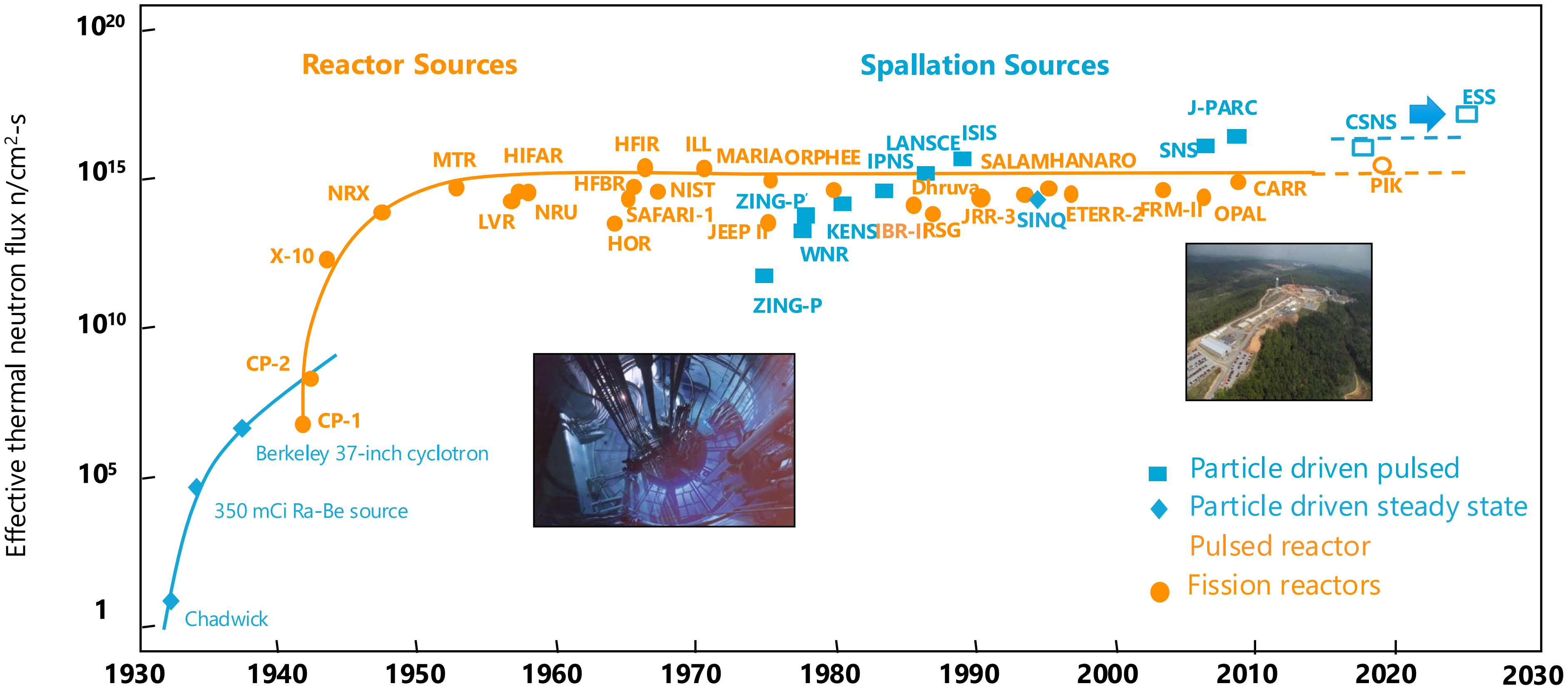




Tungsten is:
- Stable
- Abundant
- Has the right mechanical and thermal properties.

Source development

Neutron Science is intrinsically intensity limited. As most experiments require wavelength discrimination a pulsed source has intrinsic advantages.



(Updated from *Neutron Scattering*, K. Skold and D. L. Price, eds., Academic Press, 1986)

n/MW/s:

Fission: 7×10^{16}

Spallation@1GeV: 1.5×10^{17}

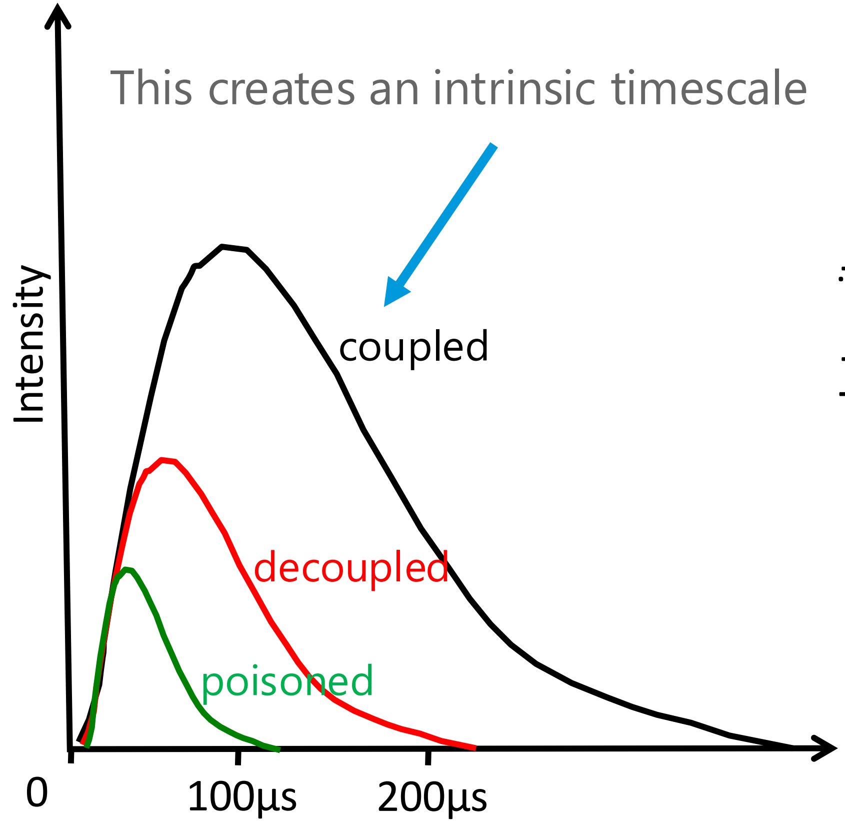
To fully exploit we require:

- high proton beam power and
- a time structure that is adapted to the neutron moderation time.

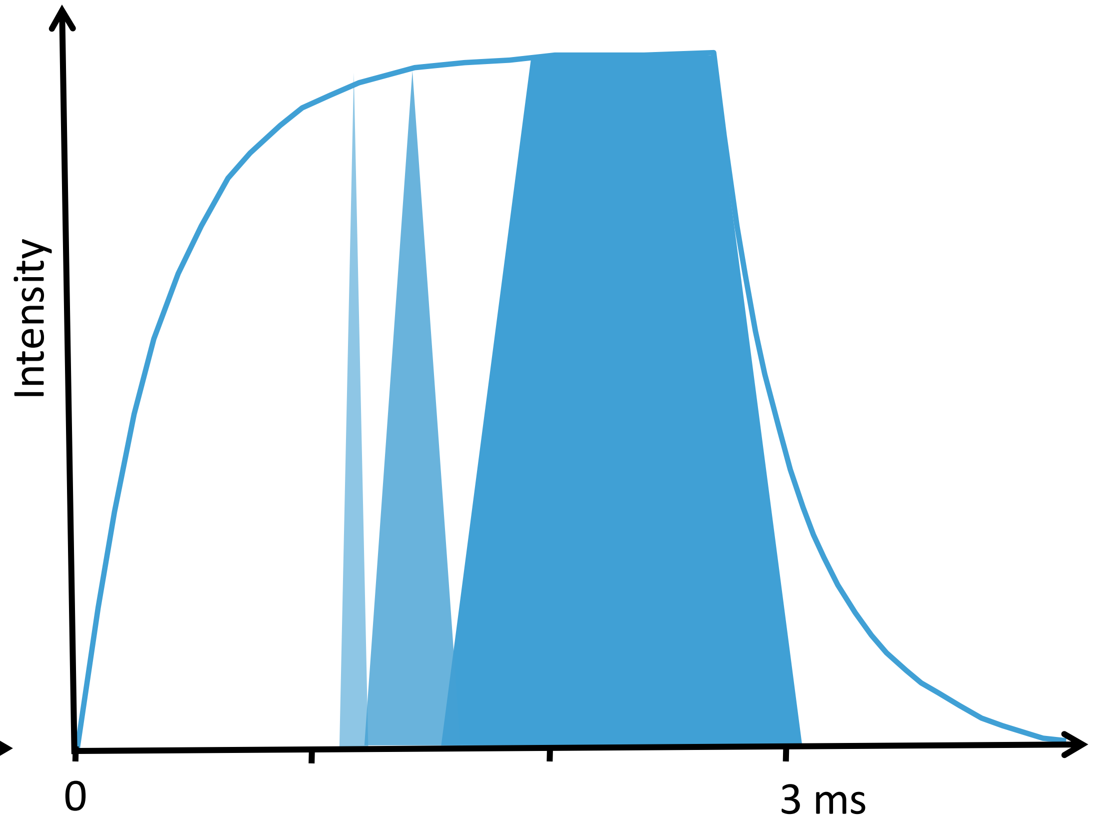
Source development

What pulse length do we want?

Short-Pulse Source
Pulse width determined by moderator



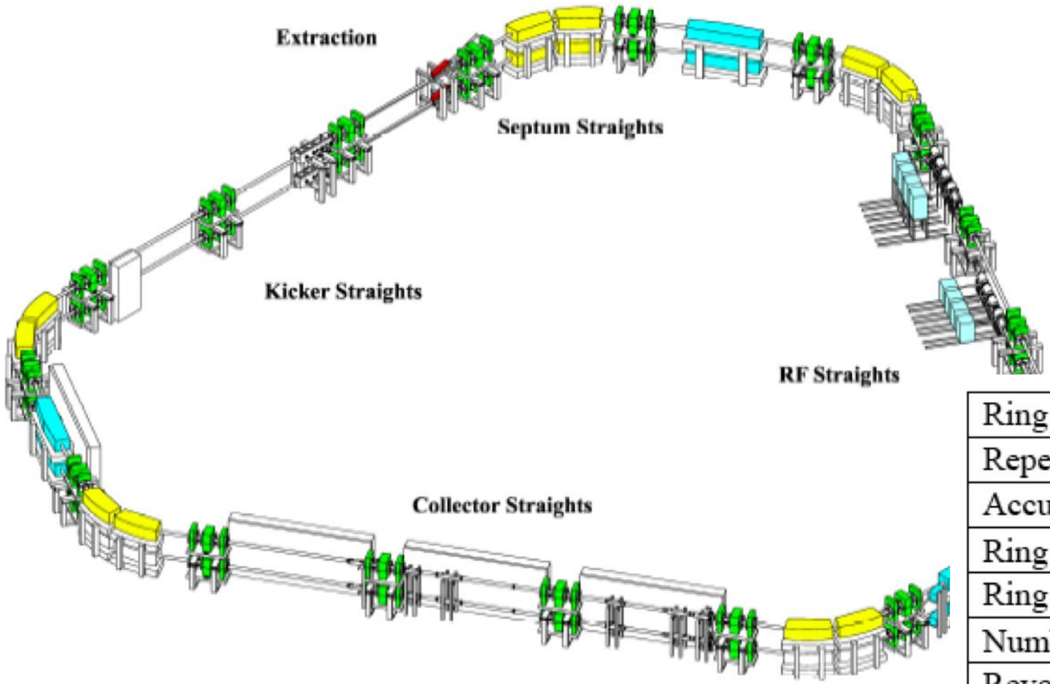
Long-Pulse Source
Pulse width determined by pulse shaping choppers



A prototypical short pulse source

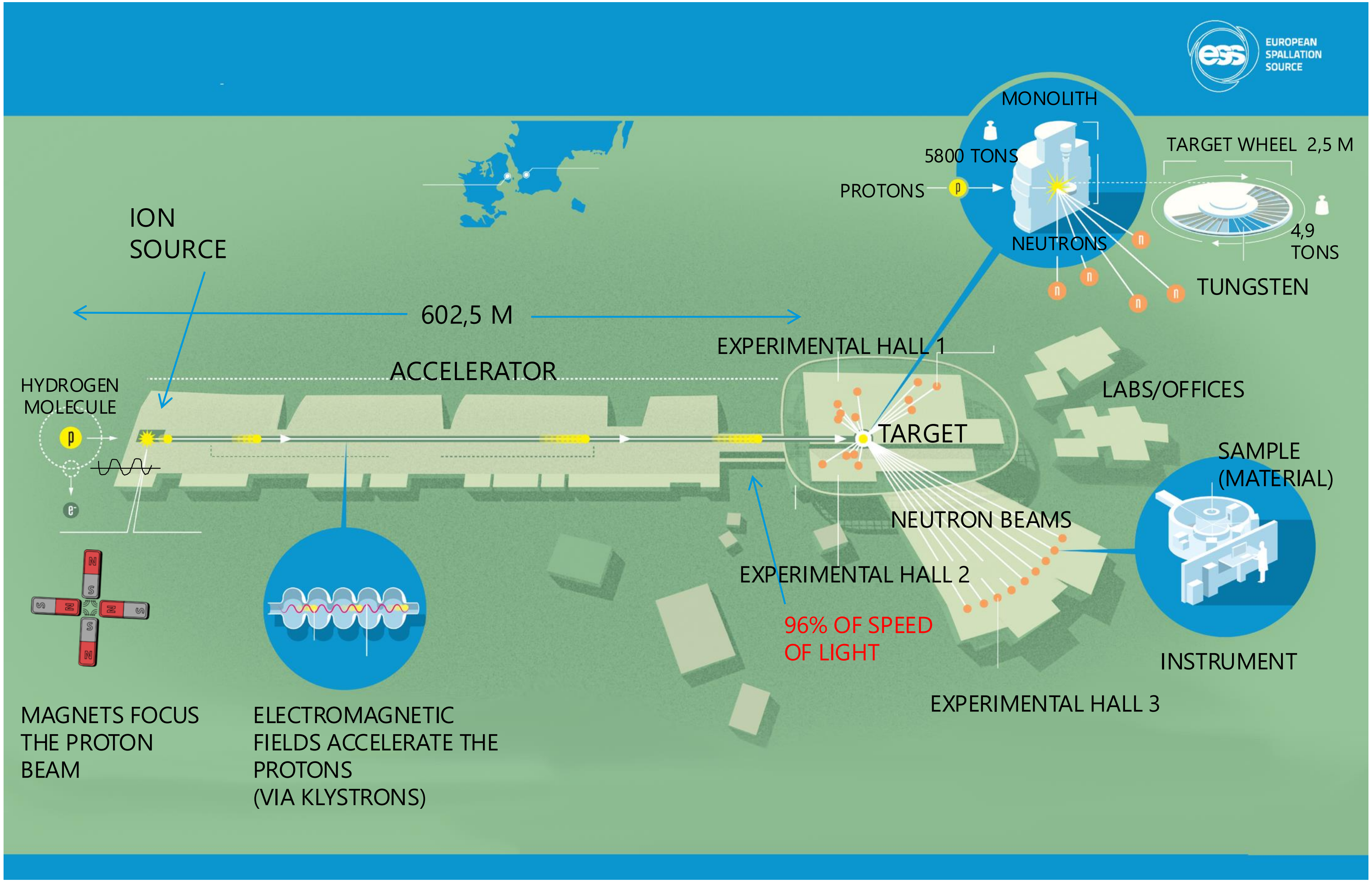
Spallation Neutron Source in Oakridge

The problem is not to create too short a pulse

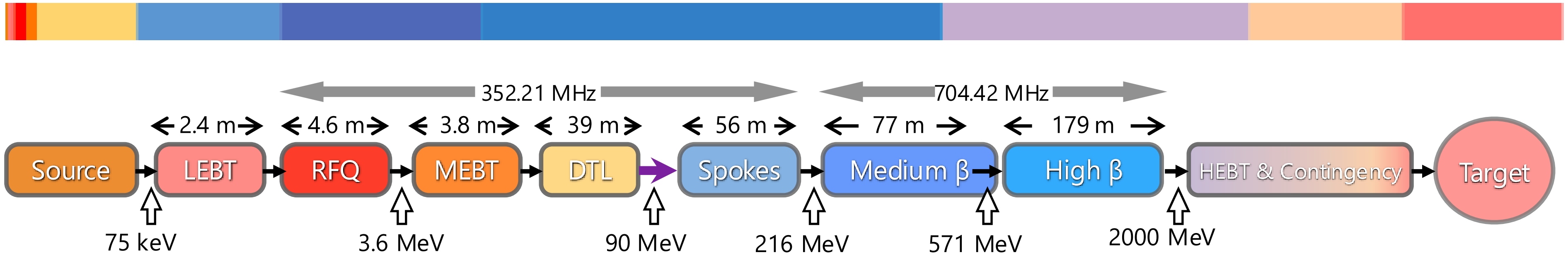


Ring max. kinetic energy (MeV)	1334.0
Repetition frequency (Hz)	50.0
Accumulator ring mean radius (m)	35.0
Ring rms unnorm. emittance (π µrad m)	30.0
Ring average circulating current (A)	46.55
Number of circulating protons ($\times 10^{14}$)	2.34
Revolution frequency (MHz)	1.2416
Main (h) & additional harmonic number	1,2
Peak kV/turn at injection	8 to 26
Ratio V(2h) / (V(h) at injection	0.4 to 0.9
Peak kV/turn during storage	26.0 to 28.0
No of 'h' cavities/ring	3 (single gap)
No of '2h' cavities/ring	1 (double gap)
Length of 'h' and '2h' cavities (m)	1.5, 2.2
Bunch and pulse extent at target (µs)	0.6, 1.4

The ESS bet: a long-pulse source

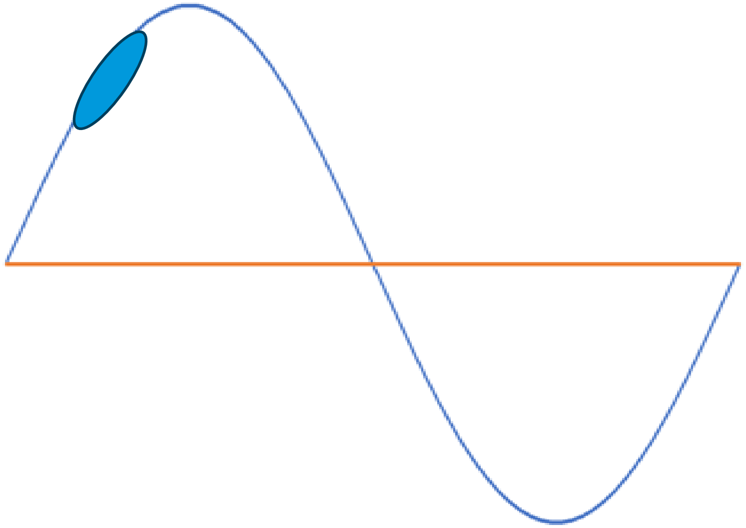


We use different structures to efficiently accelerate the beam of protons



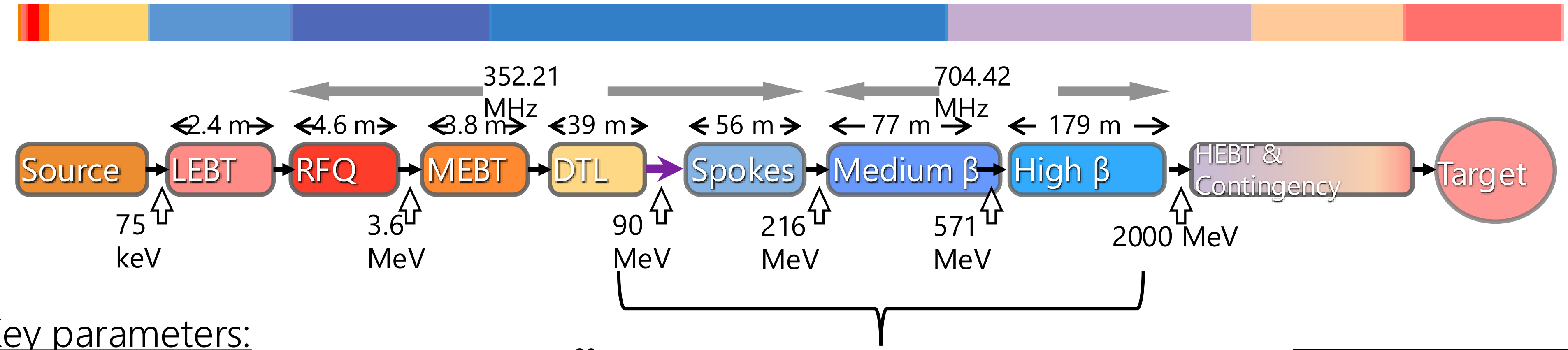
Acceleration of "bunches" of ~1 billion protons is done by rapidly oscillating electric fields with periods of 2,84 ns or 1,42 ns in almost 900 "gaps"

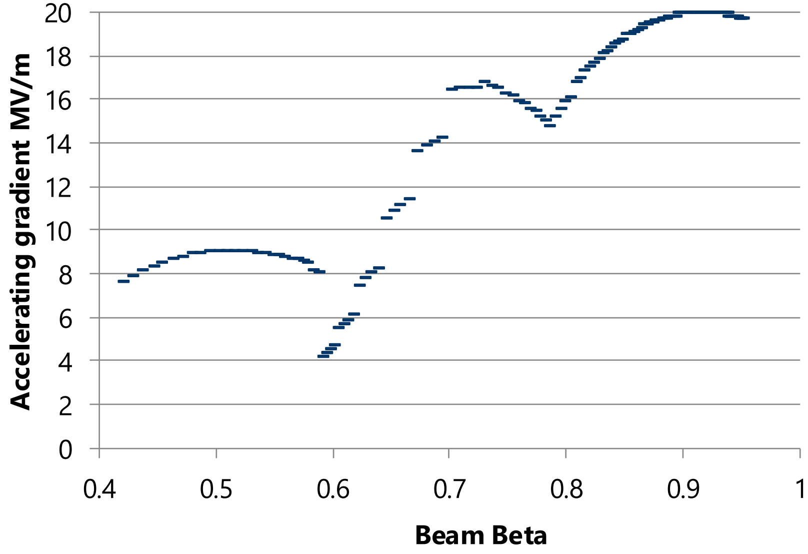
Room Temperature



2 Kelvin in cryomodule

ESS linear accelerator layout





Style	Spoke	Medium-β	High-β
Freq. (MHz)	352.21	704.42	704.42
Cavity #	26	36	84
Velocity range	0.42 to 0.58	0.58 to 0.78	0.78 to 0.95
Nom. Acc. Voltage (MV)	5.74	14.3	18.2
Loaded quality factor	2.85×10^5	8×10^5	7.6×10^5

Key parameters:

Long term goal:

5 MW average beam power

2 GeV

62.5 mA peak

2.86 ms long pulses

14 Hz

4 % duty cycle

Staged approach:

→ 2 MW, 15 instruments

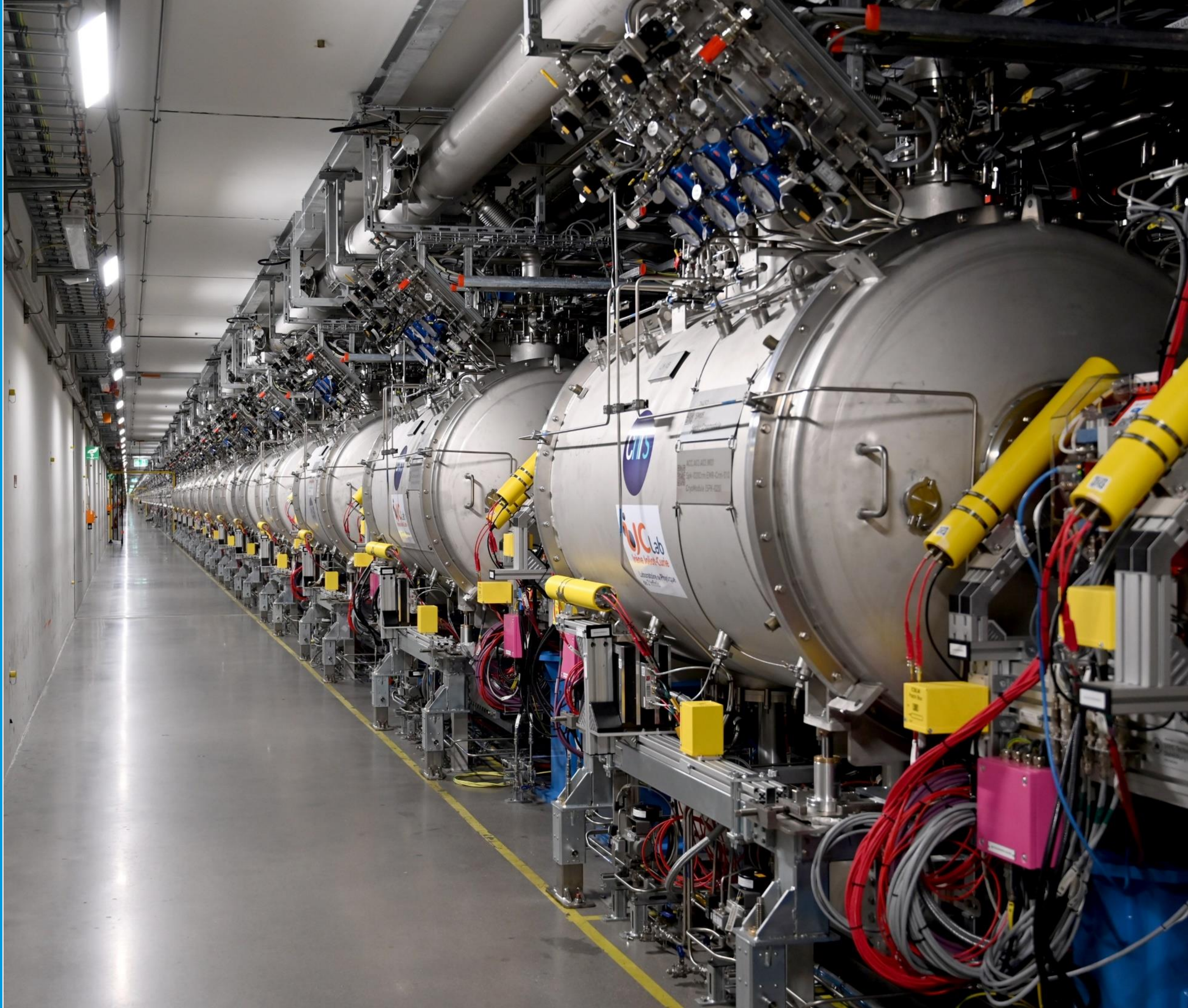
96% of acceleration will be provided by superconducting cavities supplied by dedicated high power RF sources

Accelerator

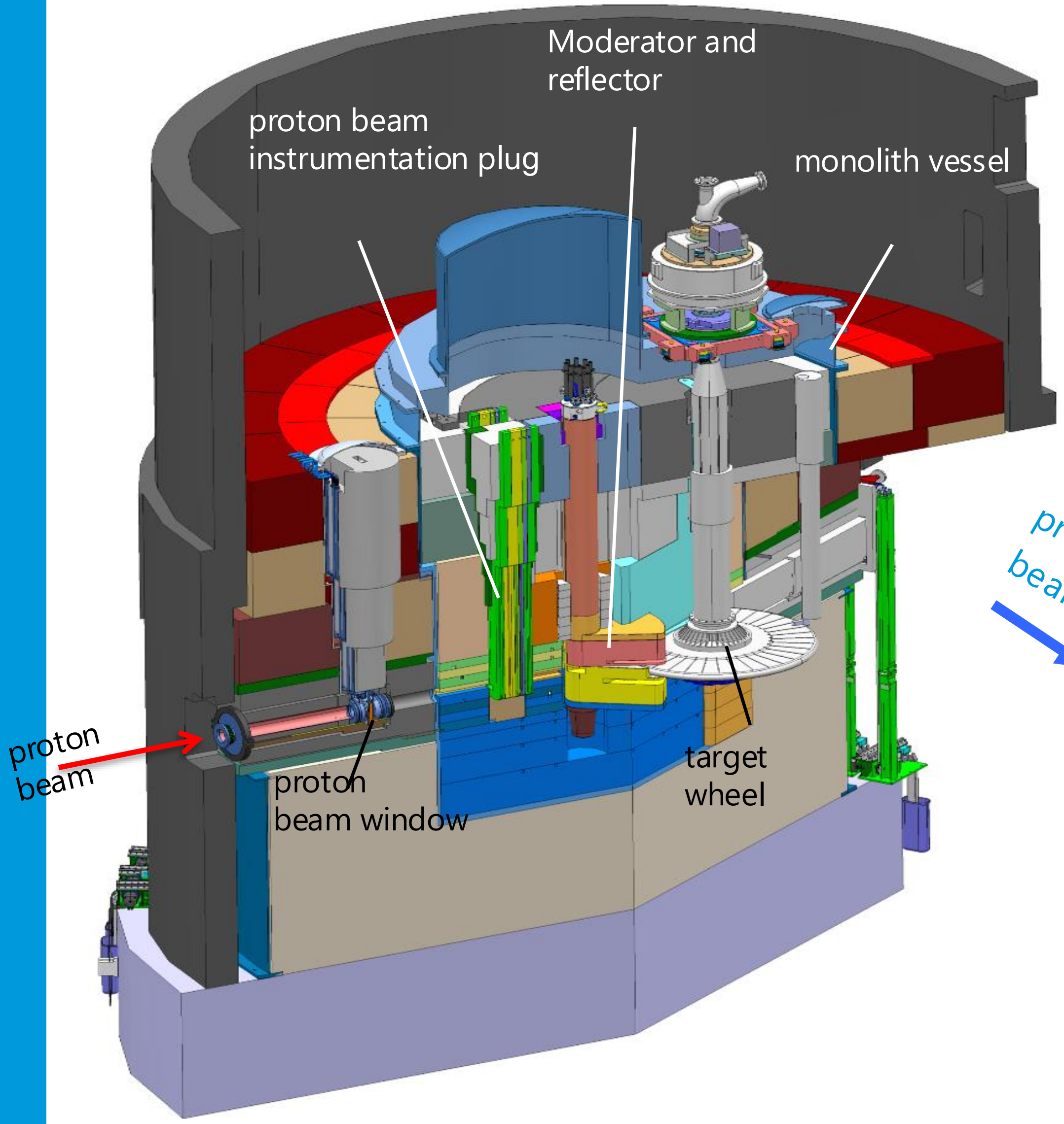
All components installed and commissioned.

Scope extended to securing 2 MW operations by having a 3 MW capability available.

Status: in operation.

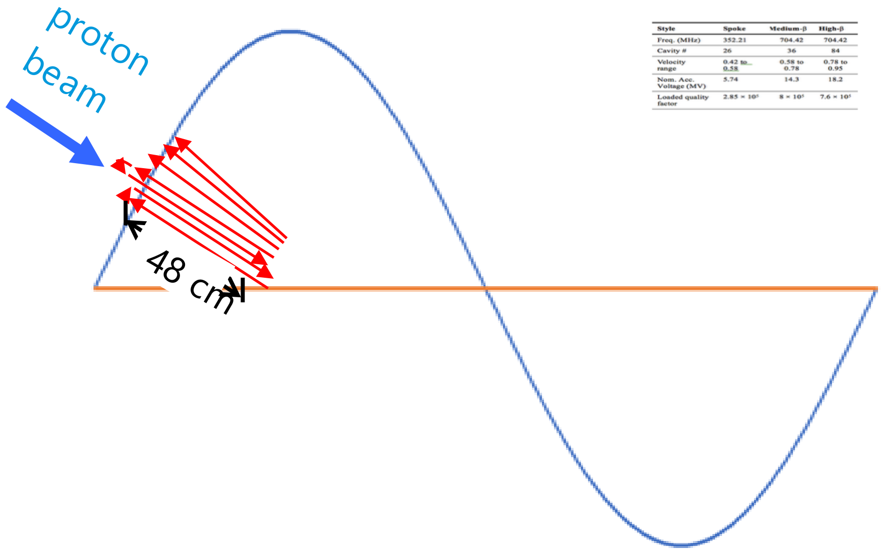


ESS Target layout



Rotating solid tungsten target

- 36 sectors
- Mass, total 11 tonnes, whereof 3 tonnes of W
- Rotates 23.3 rpm, synchronized with pulsed proton beam 14 Hz



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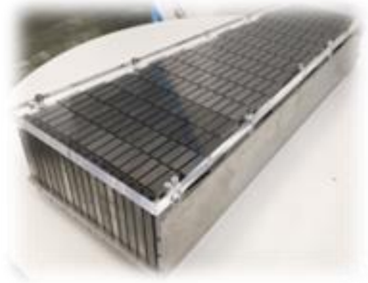
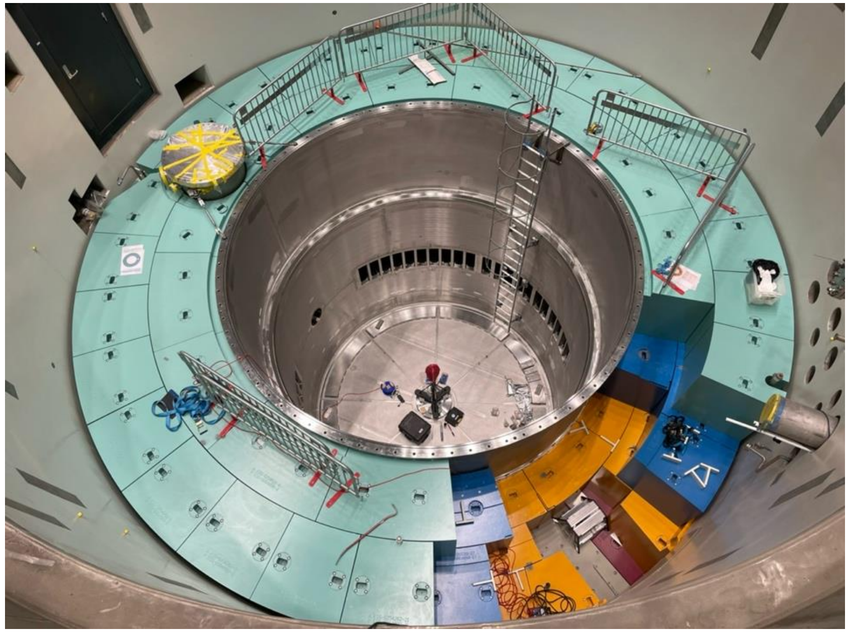
Cavity #	26	36	84
Velocity range	0.42 to 0.58	0.58 to 0.78	0.78 to 0.95
Nom. Acc. Voltage (MV)	5.74	14.3	18.2
Loaded quality factor	2.85×10^5	8×10^5	7.6×10^5

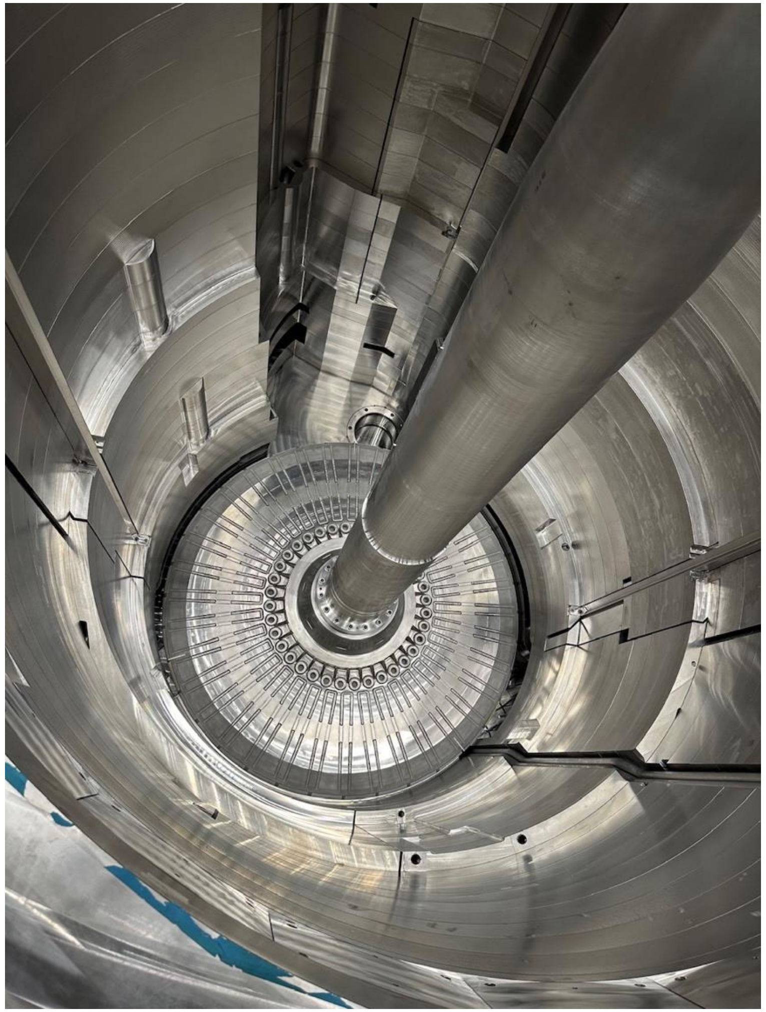
Helium cooling of target material

- Mass flow 3 kg/s
- Pressure 11 bar
- Temperature inlet/outlet 40 °C/240 °C

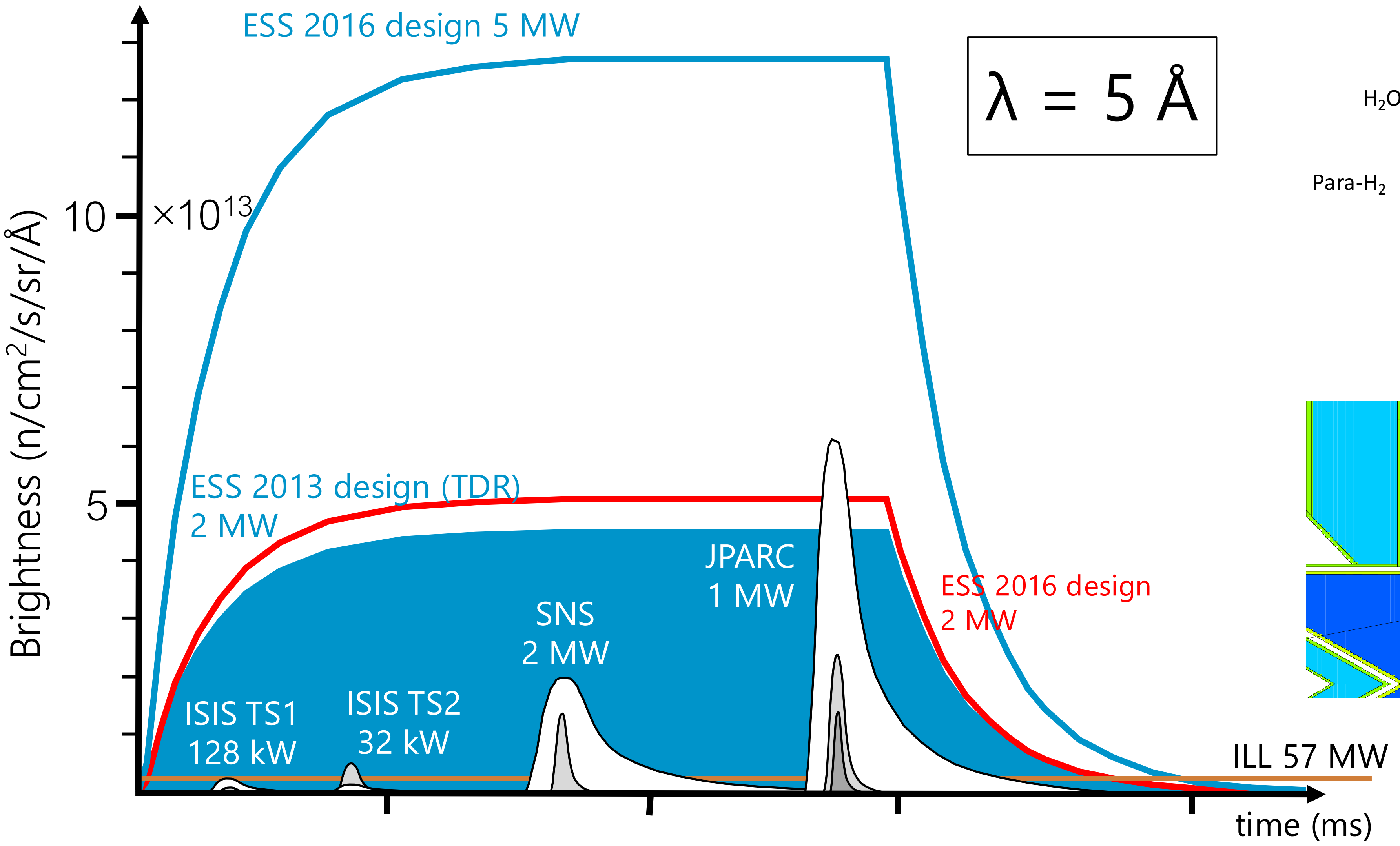


Converting a 5 MW beam of protons into beams of thermal and cold neutrons of unprecedented brilliance

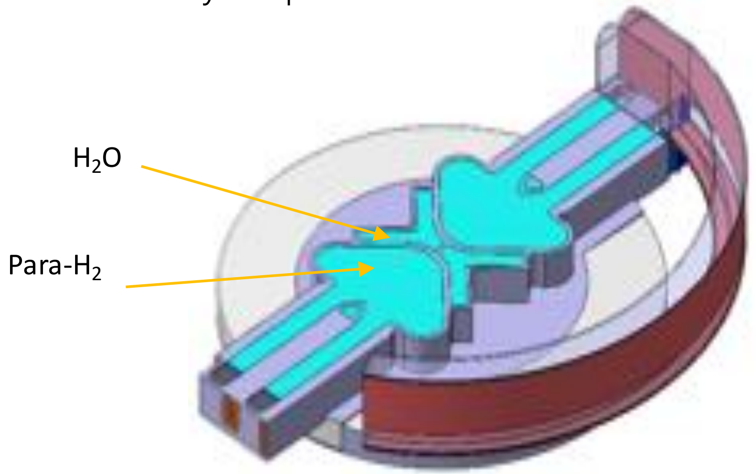


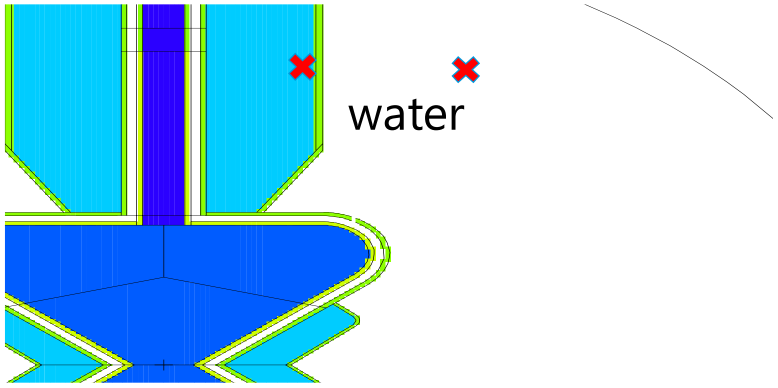


Long-pulse performance



Butterfly shape moderator





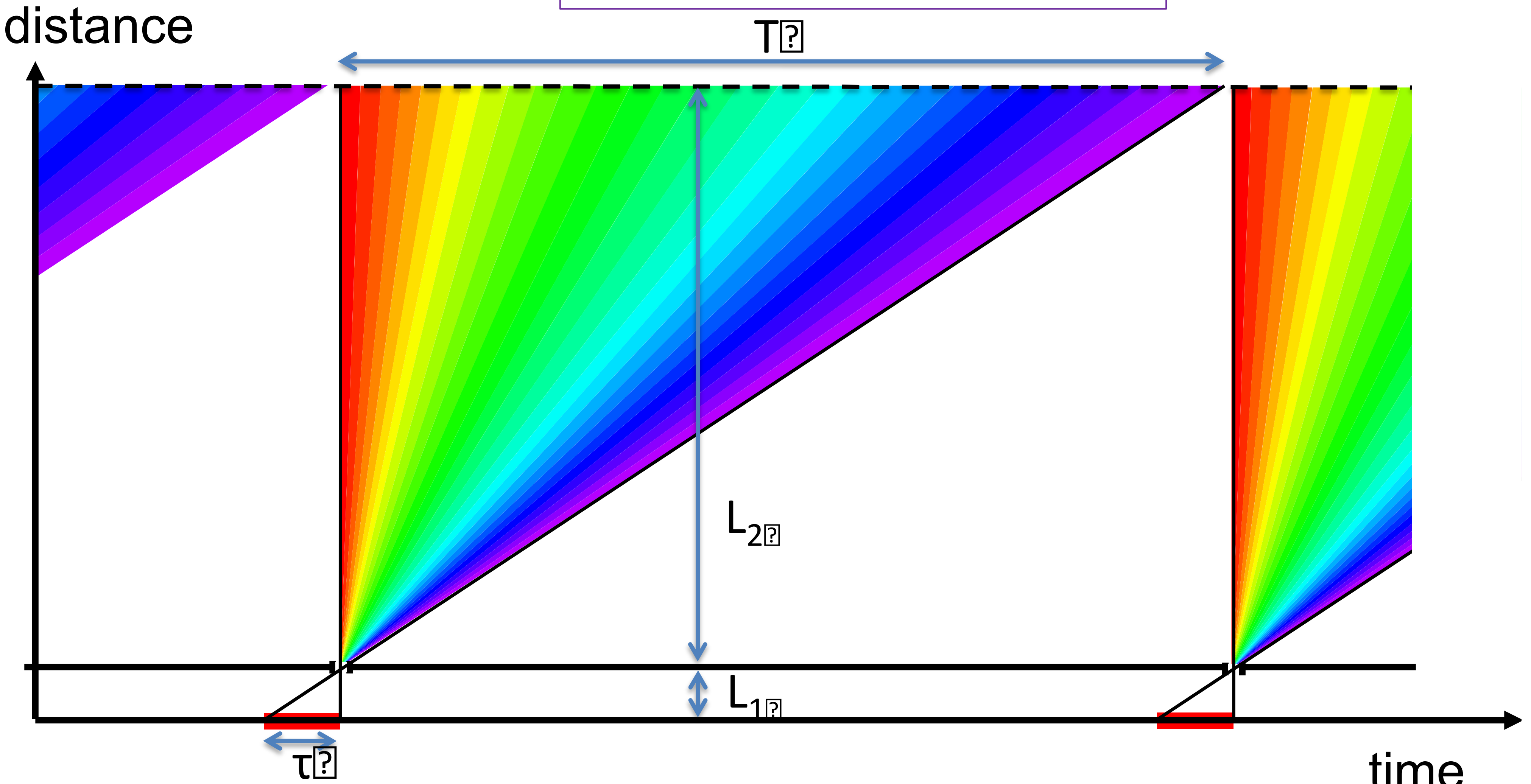
Exploiting the latest advances in the manipulation and detection of neutrons

- Life sciences
- Soft condensed matter
- Chemistry of materials
- Energy research
- Magnetism & superconductivity
- Engineering & Geo-sciences
- Archeology & Heritage conservation

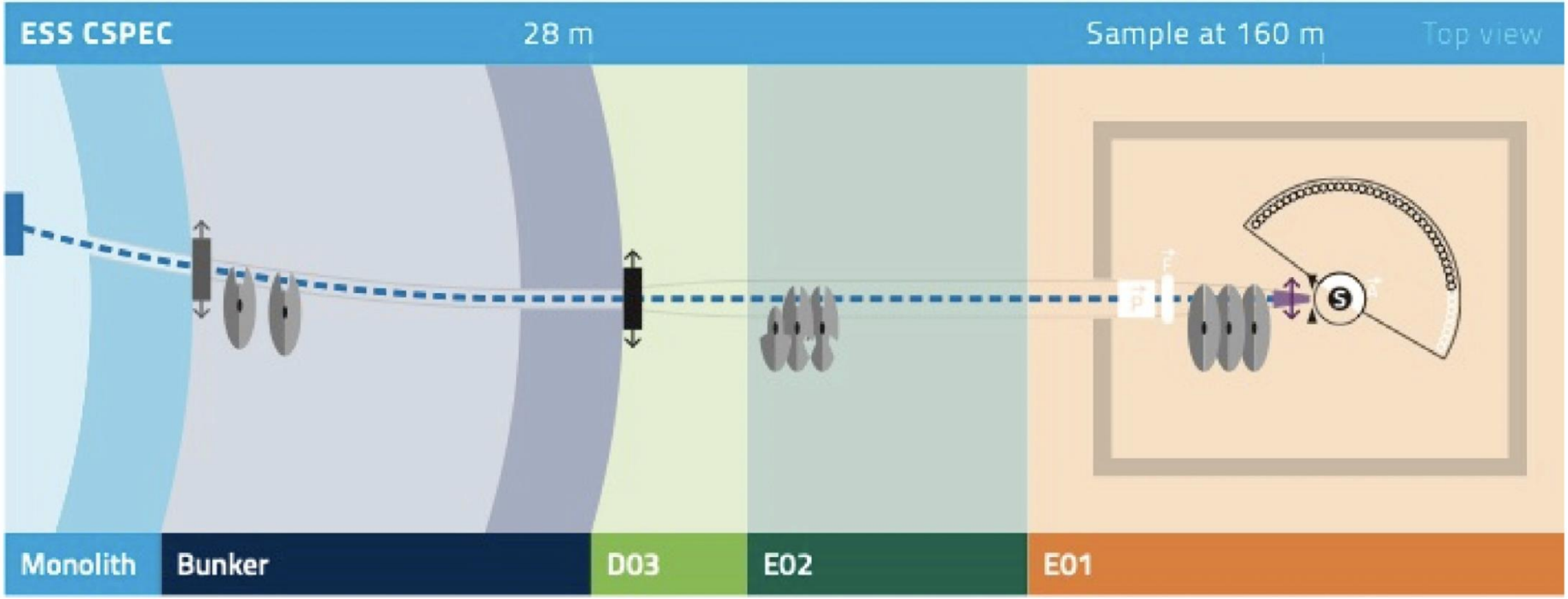
ESS Target building layout

$T/\tau = 25 \Rightarrow L_2/L_1 = 25$

$L_1 = 6.3\ \text{m} \Rightarrow L_2 = 157.5\ \text{m} \Rightarrow \Delta\lambda = 1.8\ \text{Å}$

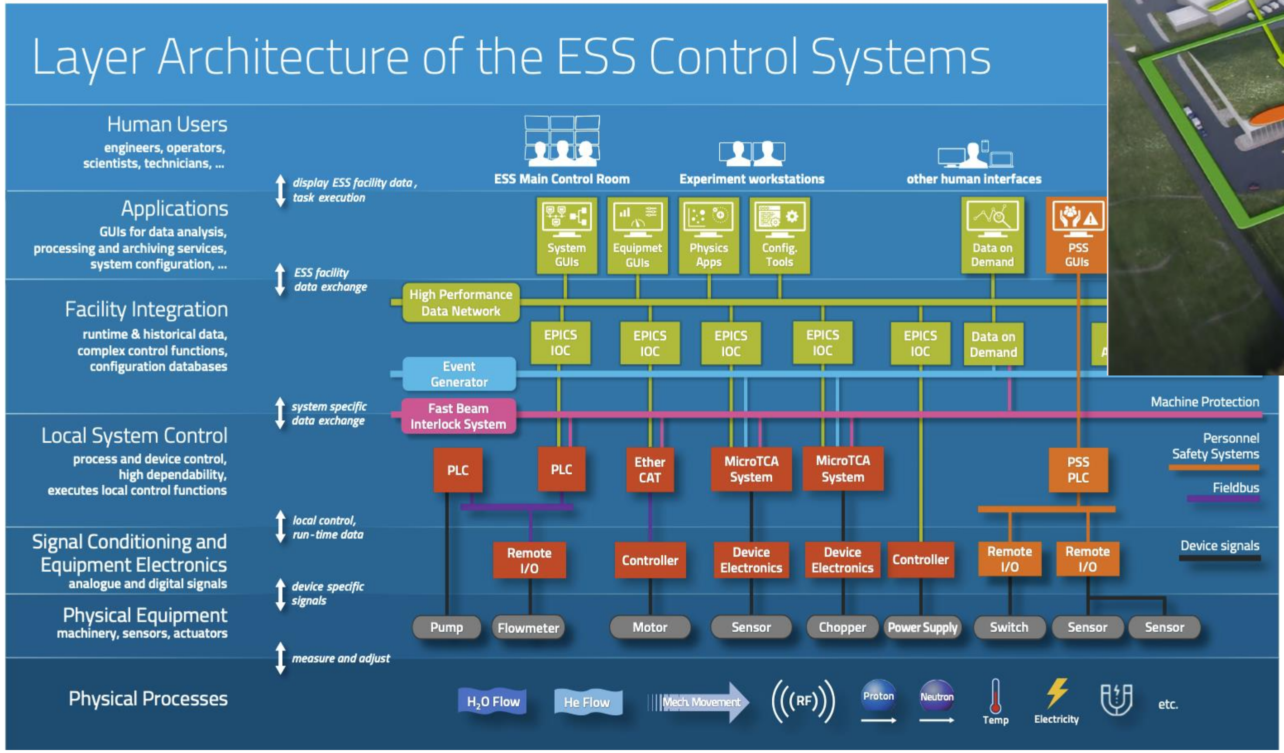


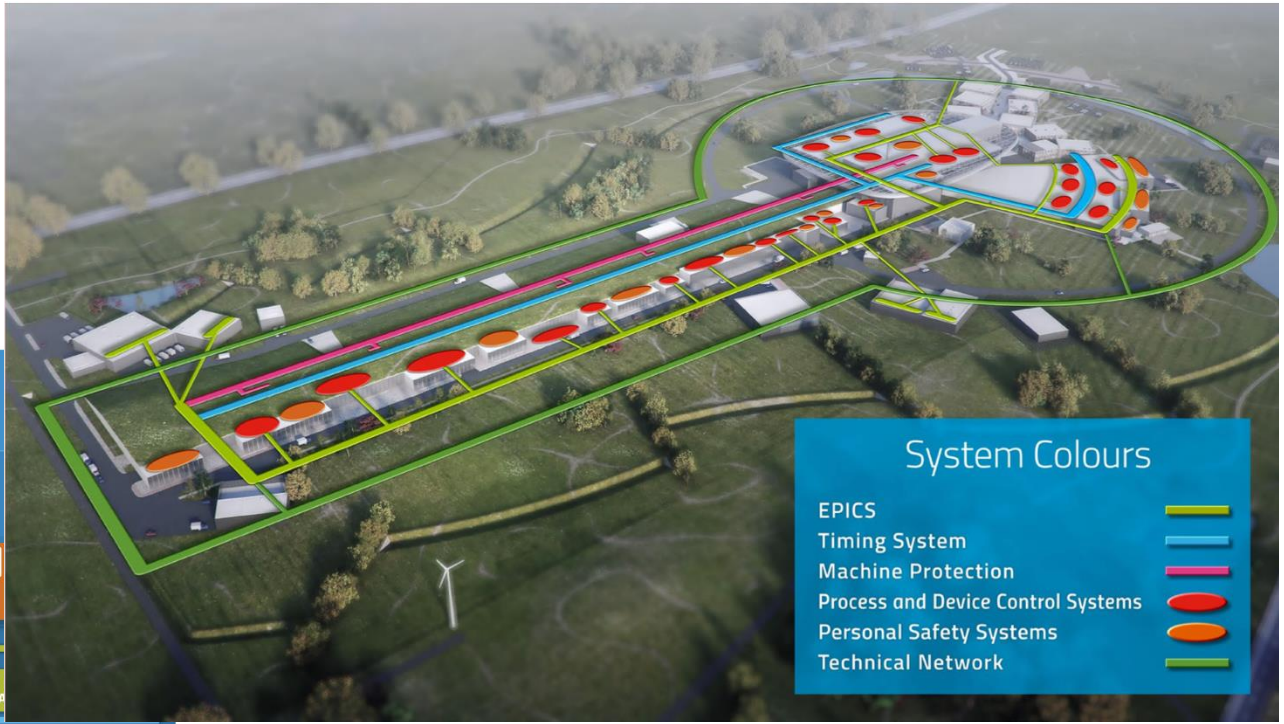
A typical instrument: CSPEC



Exploiting all possible advances in controls

Integrate latest evolution while providing maximum reliability





Exploiting all possible advances in controls

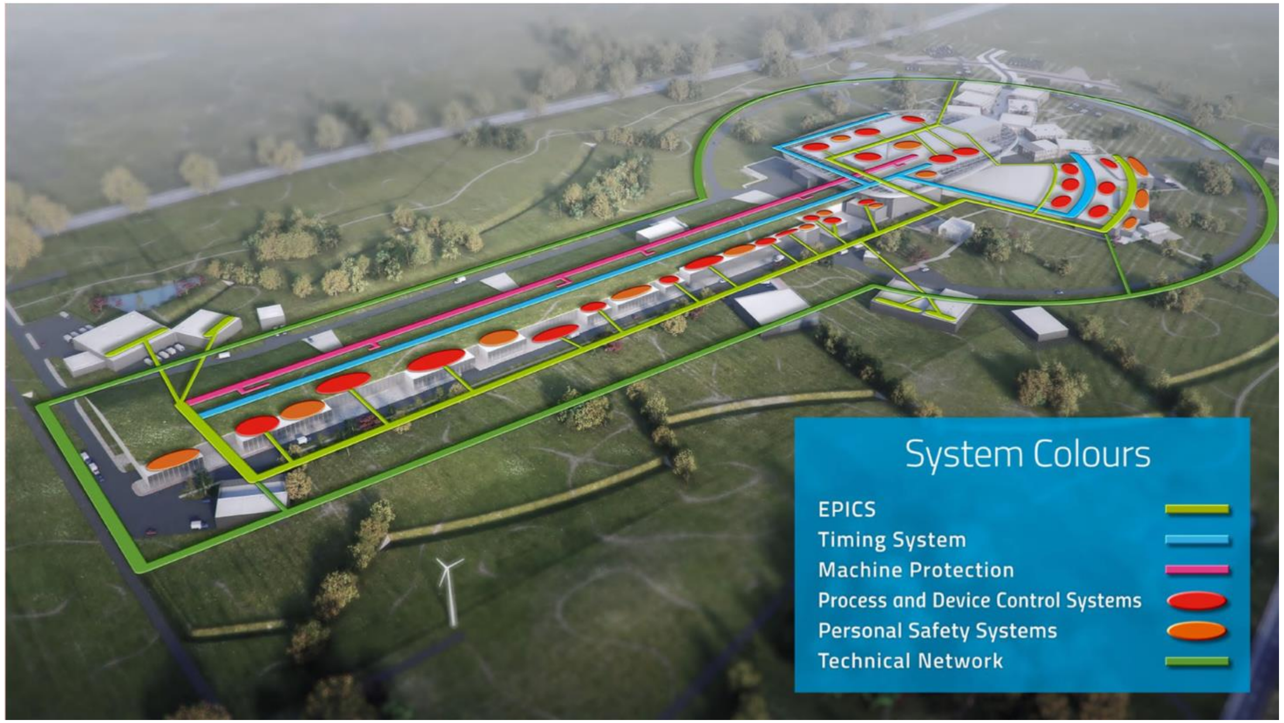
Integrate latest evolution while providing maximum reliability

Why controls are so important.

What the user wants first of all is reliability.

What is not even to be discussed is safety.

In a complex highly interconnected system of components this requires absolutely outstanding robustness of the controls.



Opening-up the World of Materials