Neutrons :
A Natural Tool for Researchers

Lecture Series : Photons and Neutrons in the Quest to Solve Societal Challenges
African School of Fundamental Physics and Applications

PRESENTED BY ANDREW JACKSON
// GROUP LEADER INSTRUMENT SCIENTISTS
// ACTING HEAD NEUTRON INSTRUMENTS DIVISION

2021-01-12

Context

Part A: Synchrotron and neutron based diffraction and spectroscopic techniques

Part B: Large Research Infrastructure as tools for innovation

January 12 :

- **Neutrons: A Natural Tool for Researchers // Andrew Jackson**

January 19 :

- Neutron scattering as a tool to understand quantum magnetism: Magnetism and the ESS // Pascale Deen

January 26 :

- Non-destructive testing with neutrons: Engineering materials and components revealed // Robin Woracek

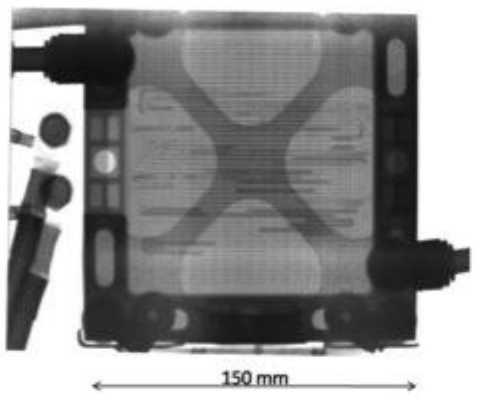
February 2 :

- Fundamental physics possibilities with neutrons at the European Spallation Source // Valentina Santoro

Why Neutrons?

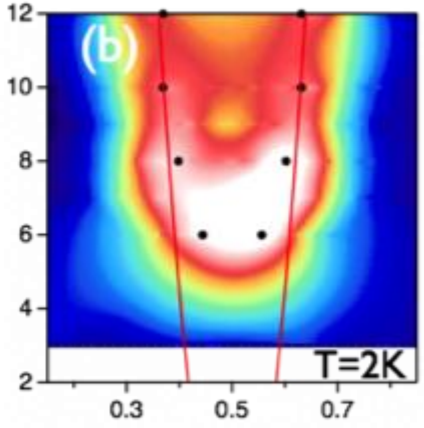
Neutrons have special properties …

Charge neutral
Deeply penetrating



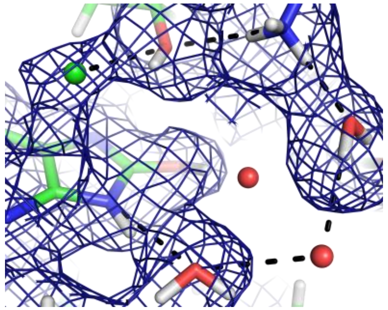
Hydrogen and water distribution in fuel cells

Magnetic moment (spin)
Probe of magnetism



Understanding supercondutors

Nuclear scattering
Sensitive to light elements and isotopes



Understanding drug binding and enzyme action

X-Rays and Neutrons

Discovered by Wilhelm Röntgen in 1895 during studies on cathode ray tubes.

In 1901 Röntgen was awarded the first Nobel prize in Physics for the discovery.

	X-Ray	Neutron
Mass	None	1.674928 x 10^{-27} kg (1839 electrons)
Spin	1	1/2
Magnetic Moment	None	-1.9130427 μ_n
Energy	10 eV – 100 keV	0.1 meV – 0.5 eV
Wavelength	0.01 nm to 100 nm	0.01 nm to 3 nm
Source brightness	10^6 – 10^{20} (photons/mm^2/s/mrad/0.1% bandwidth)	10^{10} – 10^{14} (neutrons/cm2/s/sr/Å)

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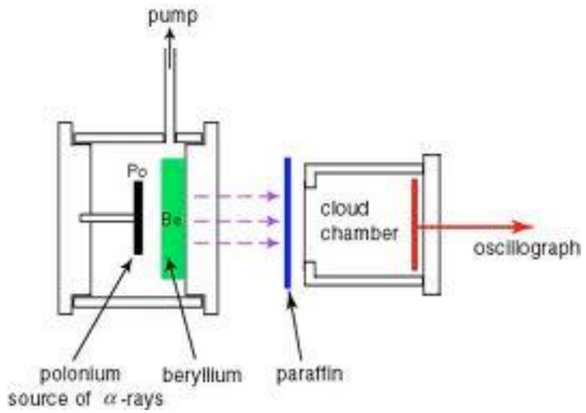
X-Rays and **Neutrons**

Discovered by James Chadwick in 1923 after prediction by Ernest Rutherford in 1920.

In 1935 Chadwick was awarded the Nobel prize in Physics for the discovery.



$^{4}_{2}He + ^{9}_{4}Be \Rightarrow ^{12}_{6}C$ + 10 neutrons

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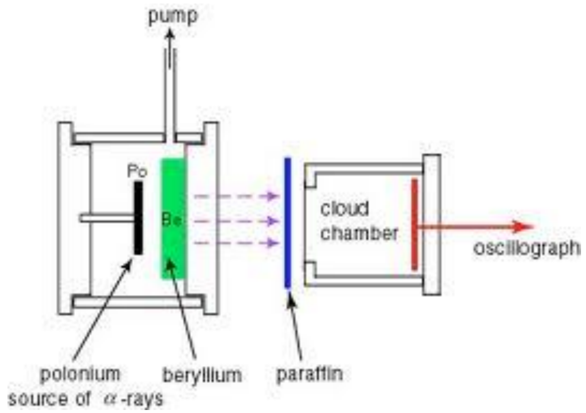

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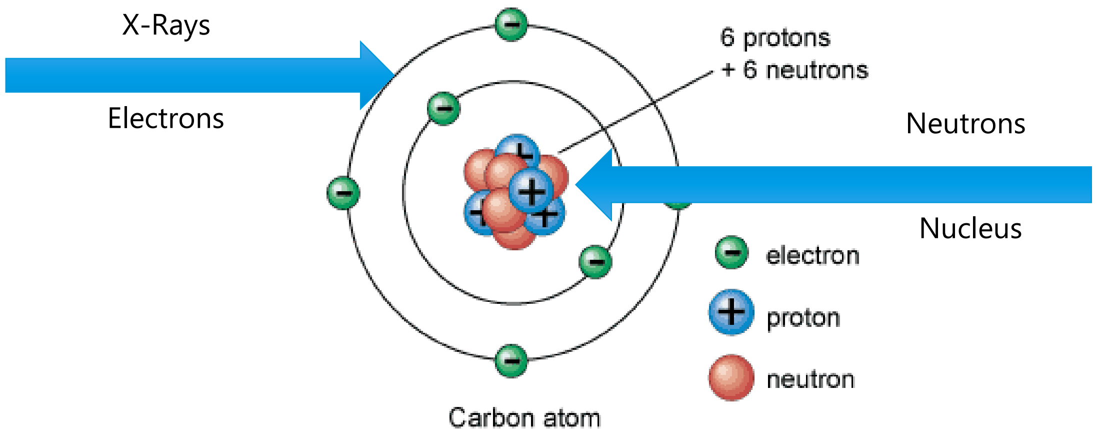
X-Rays and Neutrons

Interaction with atoms



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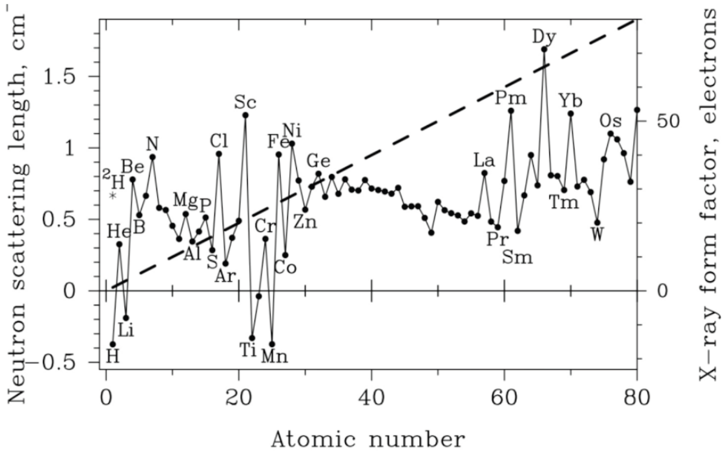
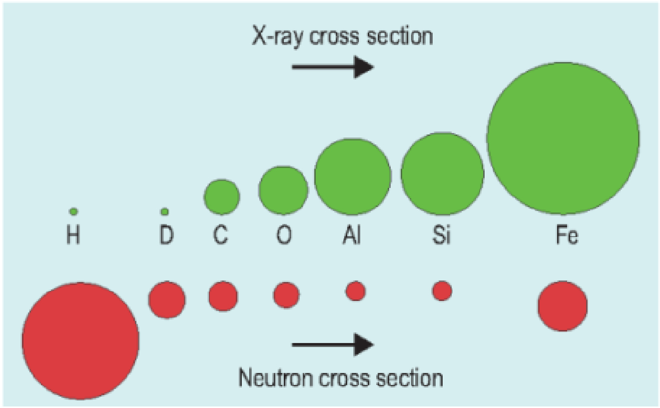
X-Rays and Neutrons

Scattering Cross Section





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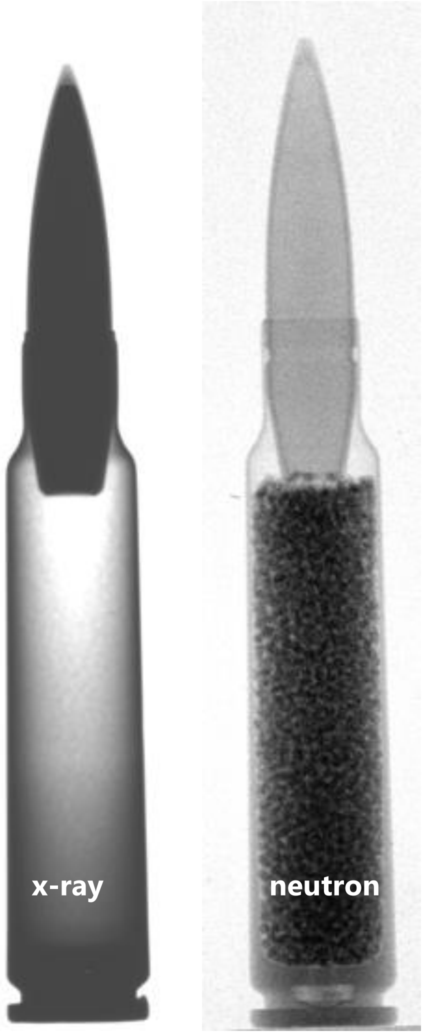
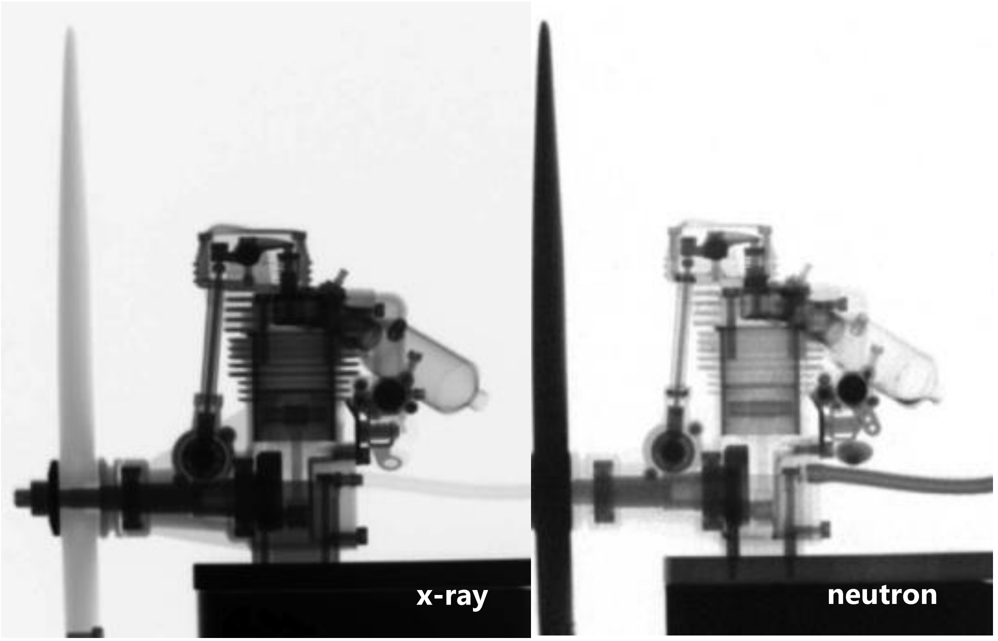
X-Rays and Neutrons

Different views of the same thing

Courtesy of the NIAG group, PSI, Switzerland.





Due to the different interaction and cross sections, neutrons and x-rays provide complementary information

X-Rays and Neutrons

Contrast and Refractive Index

When the monster came, Lola remained undetected.

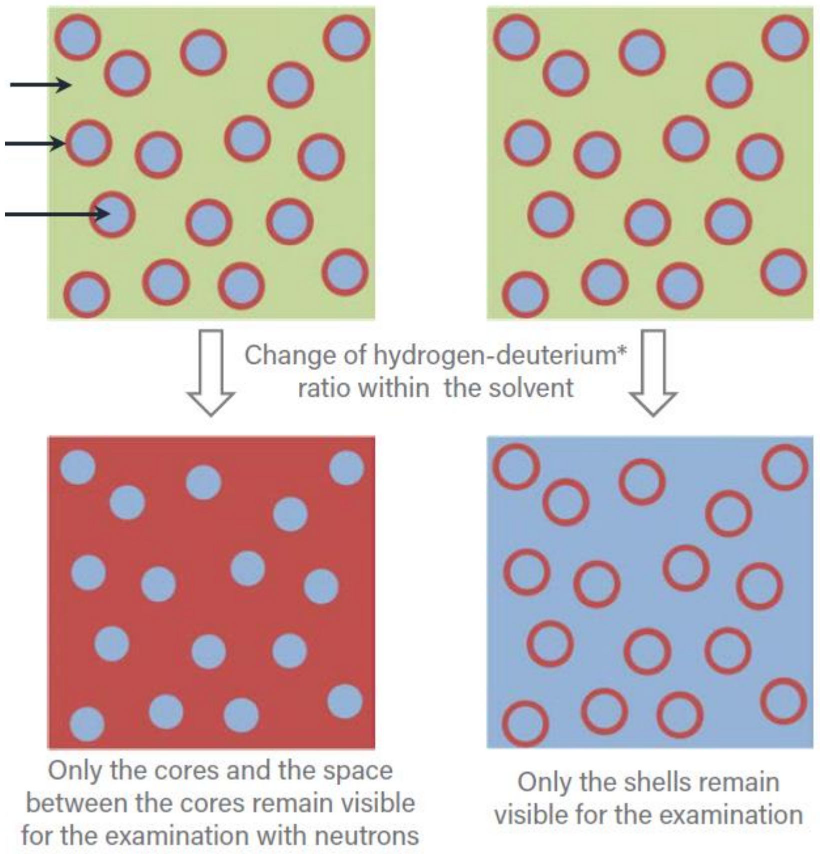
Harold, of course, was immediately devoured.

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

Combining X-Ray and Neutron measurements provides more information

X-Rays and Neutrons

Contrast and Refractive Index



I. Grillo, ILL

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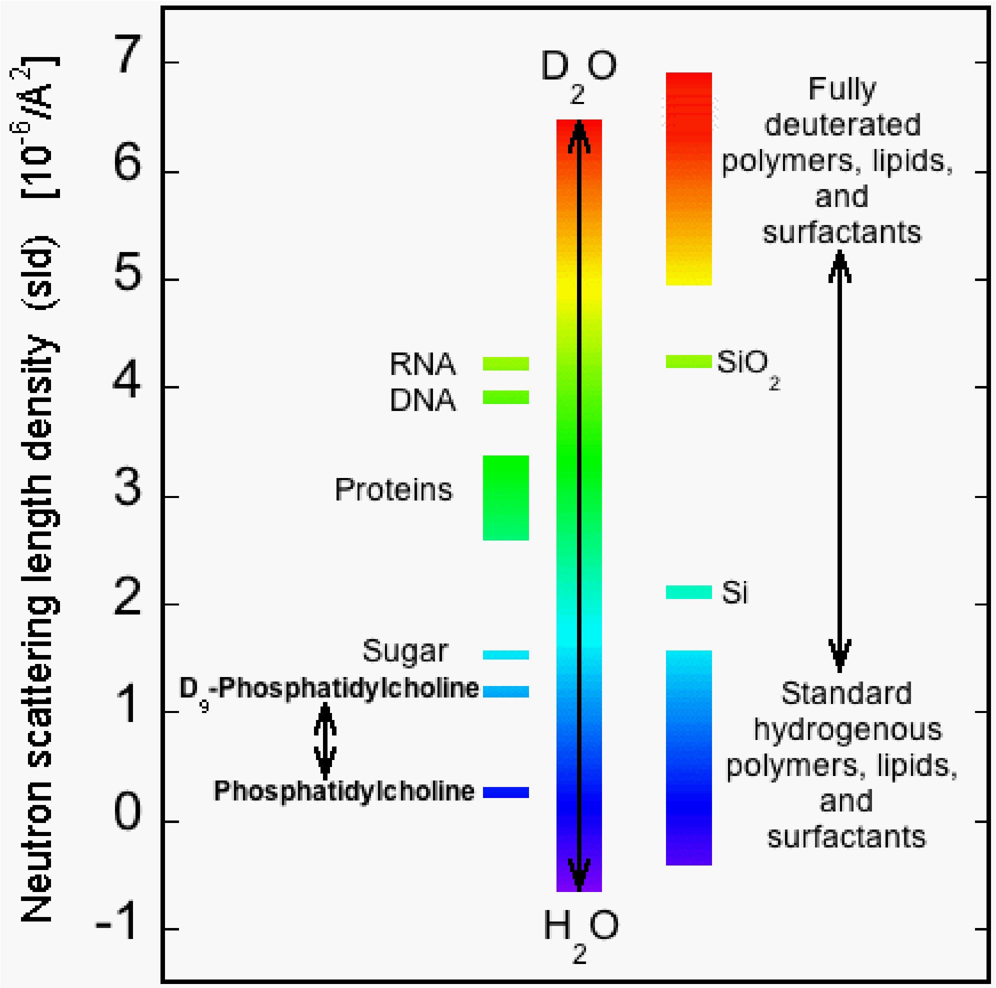
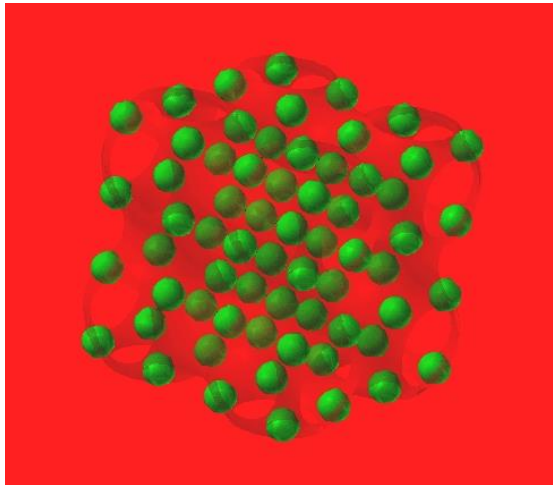
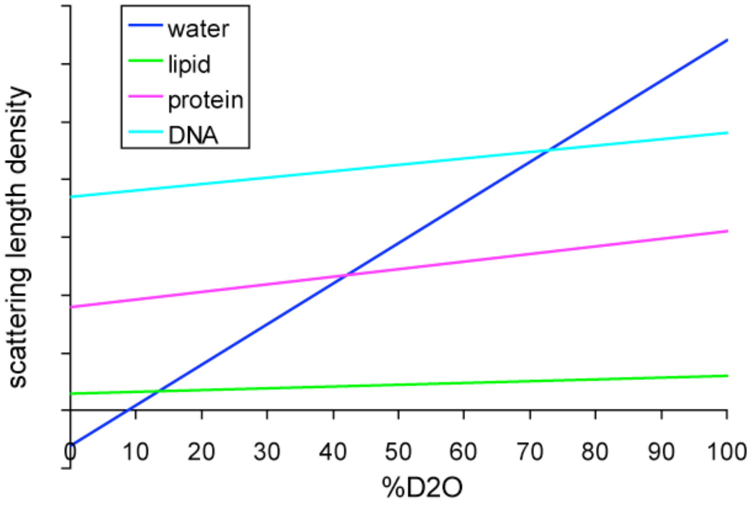
Contrast Variation in Biological Systems

The power of H/D substitution





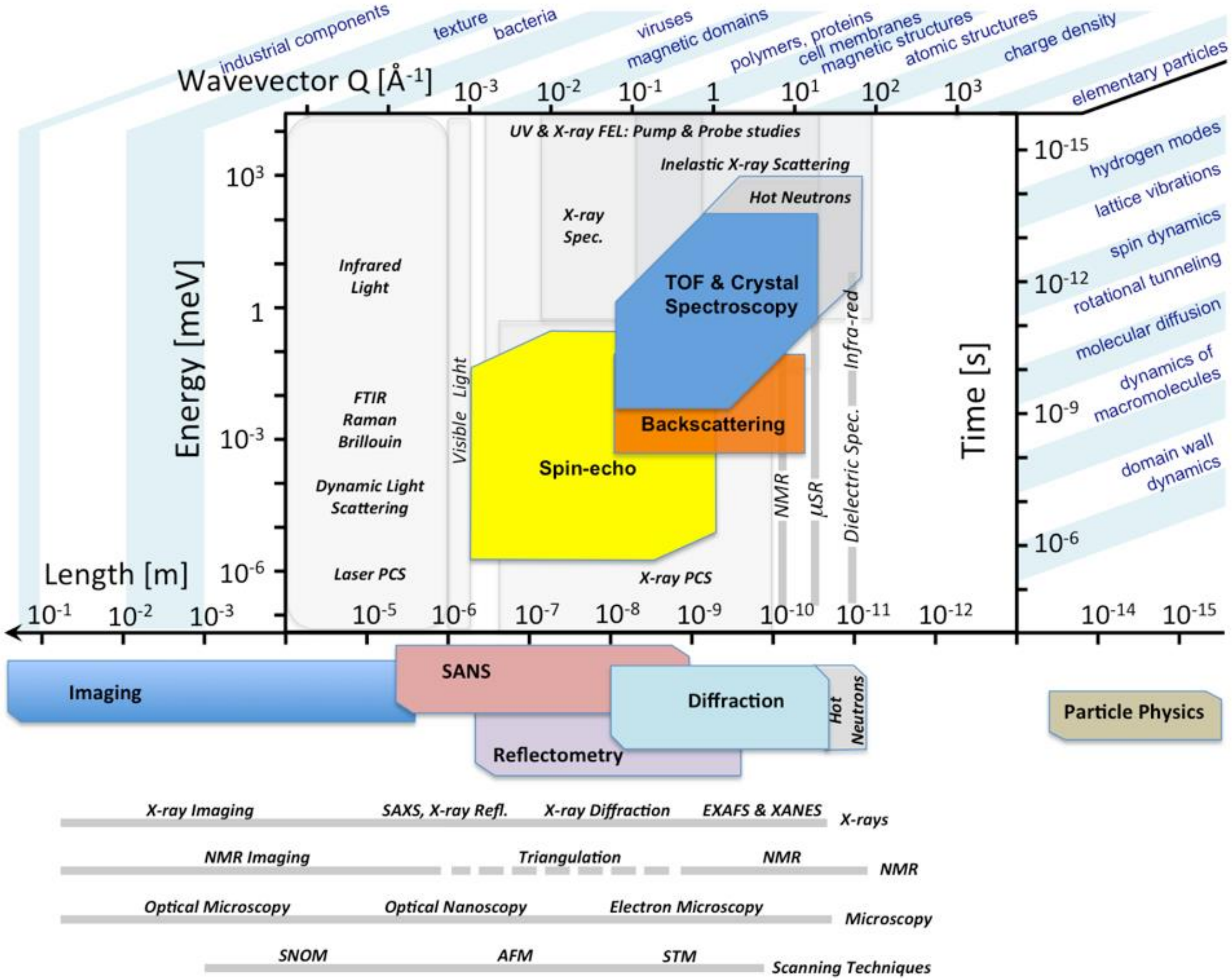


Example

- Proteins in a deuterated lipid matrix
- Changing solvent from H_2O to D_2O can mask out lipid contribution.

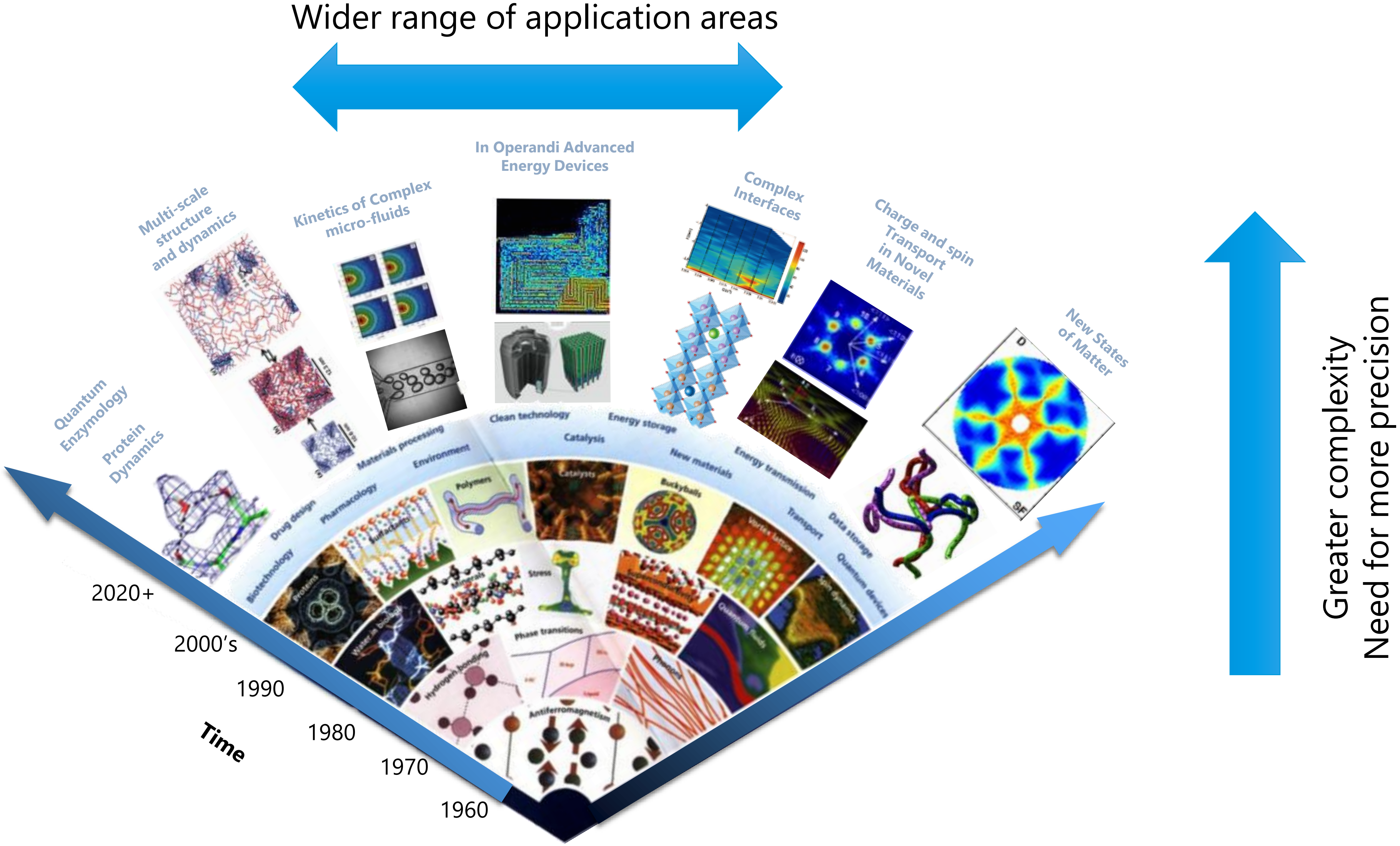
Contrast variation with stable Deuterium isotopes can selectively highlight features in biological molecules/materials

Neutron Scattering Techniques



Neutron Science Applications

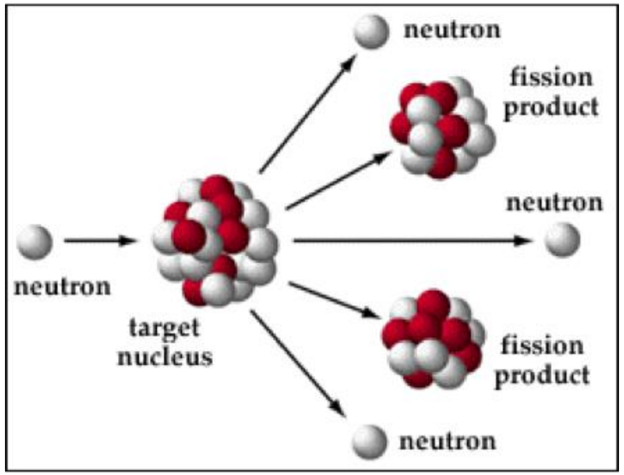
Pushing the boundaries



Generating Neutrons for Experiments

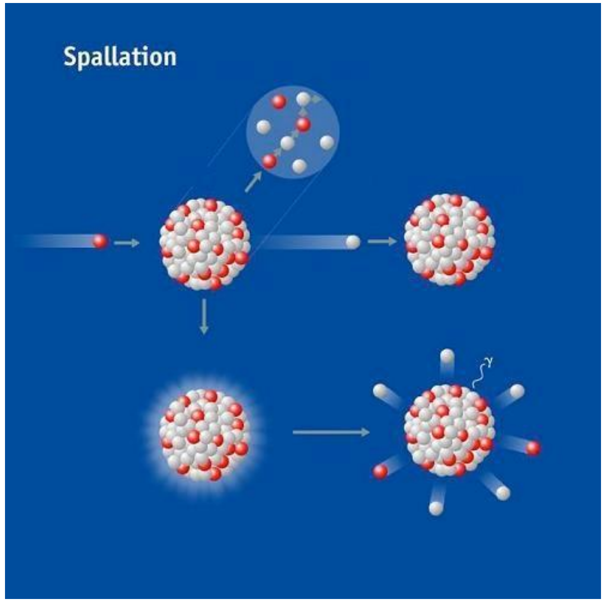
Types of source

Nuclear Fission
(Reactors)



Element (e.g. ^{235}U) that decays with neutron release and upon bombardment with a neutron then splits to release more neutrons generating a chain reaction

Spallation



A high energy pulsed proton beam is used to bombard a heavy metal target.

10 - 30 neutrons produced per proton.

Generating Neutrons for Experiments

Types of source

The neutrons generated must often be **moderated** to lower their energy (increase their wavelength) before they are used in scattering experiments

Moderation at reactor :
water, liquid hydrogen or liquid deuterium

Moderation at spallation source :
water, liquid hydrogen or solid methane

$$E = k_B T$$

Boltzmann

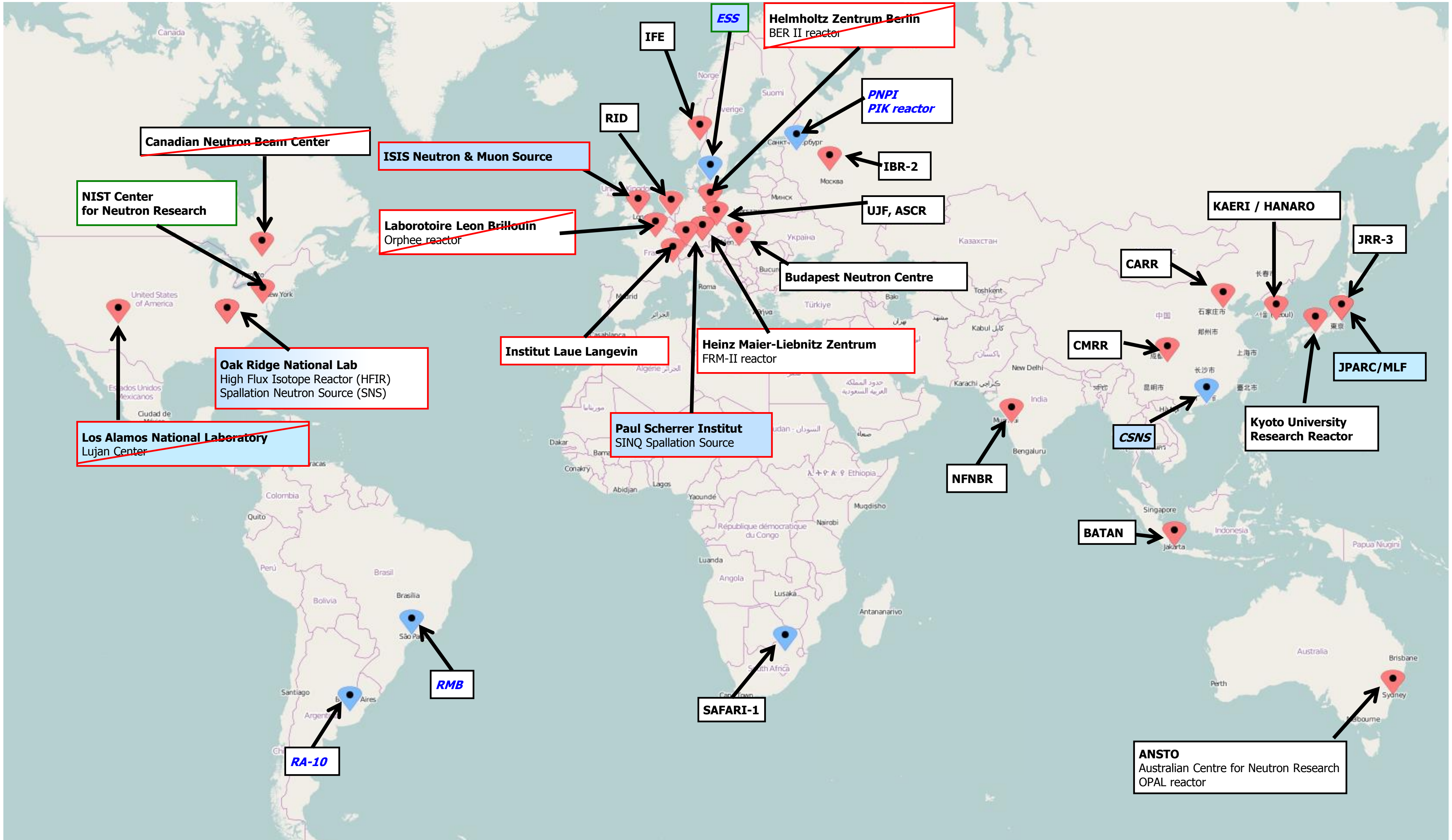
$$E = k_B T = \frac{1}{2} m v^2 = \frac{h}{2m\lambda^2}$$

$$\lambda = \frac{h}{mv}$$

De Broglie

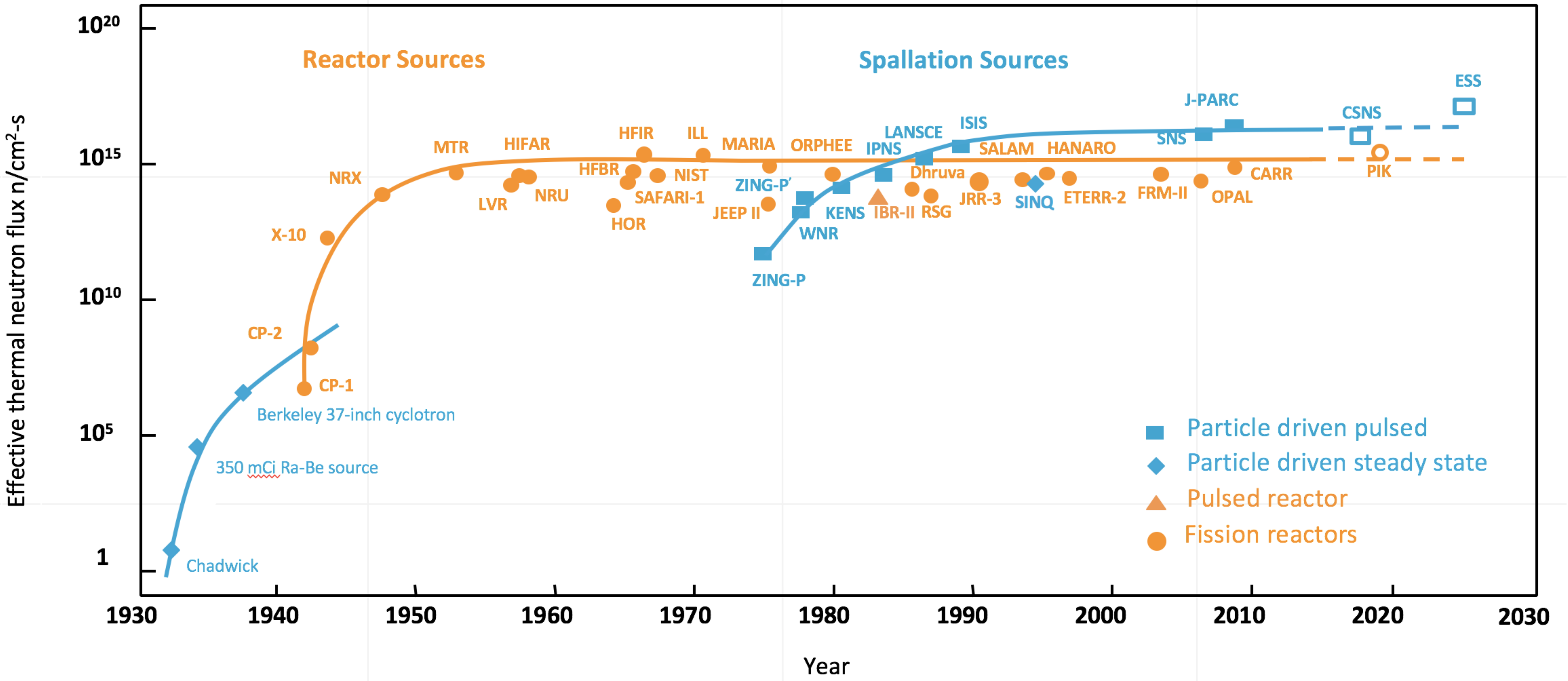
Source	Energy	Temperature	Wavelength
cold	0.1-10	1-120	30-3
thermal	5-100	60-1000	4-1
hot	100-500	1000-6000	1-0.4

Neutron Scattering Facilities



Neutron Source Brightness

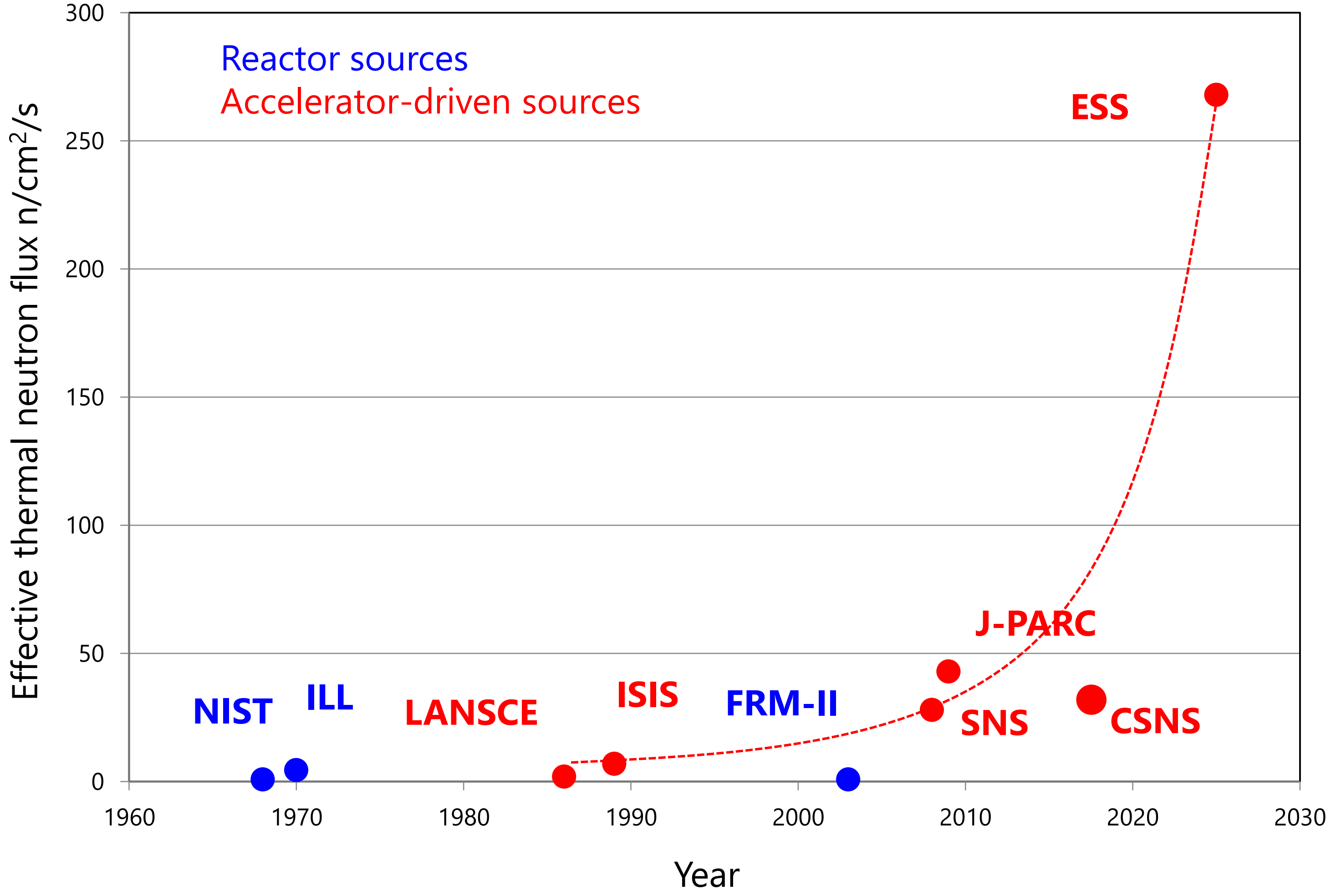
What are the limits?



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

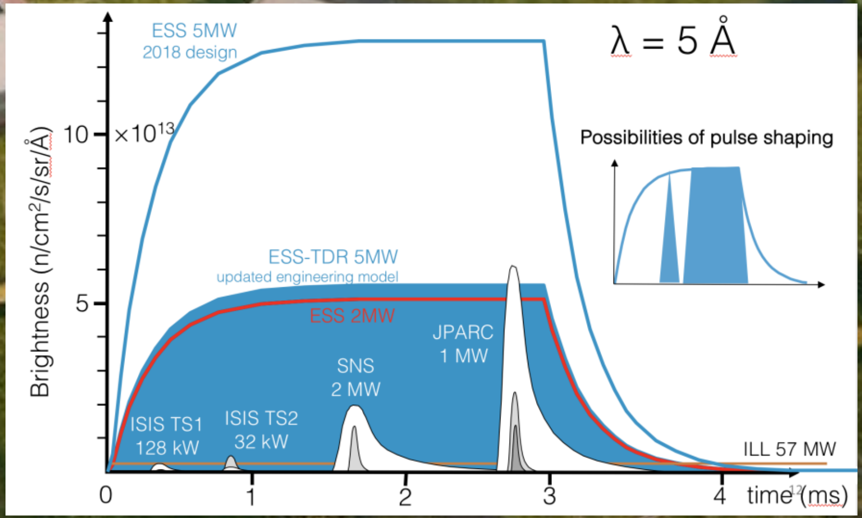
Neutron Source Brightness

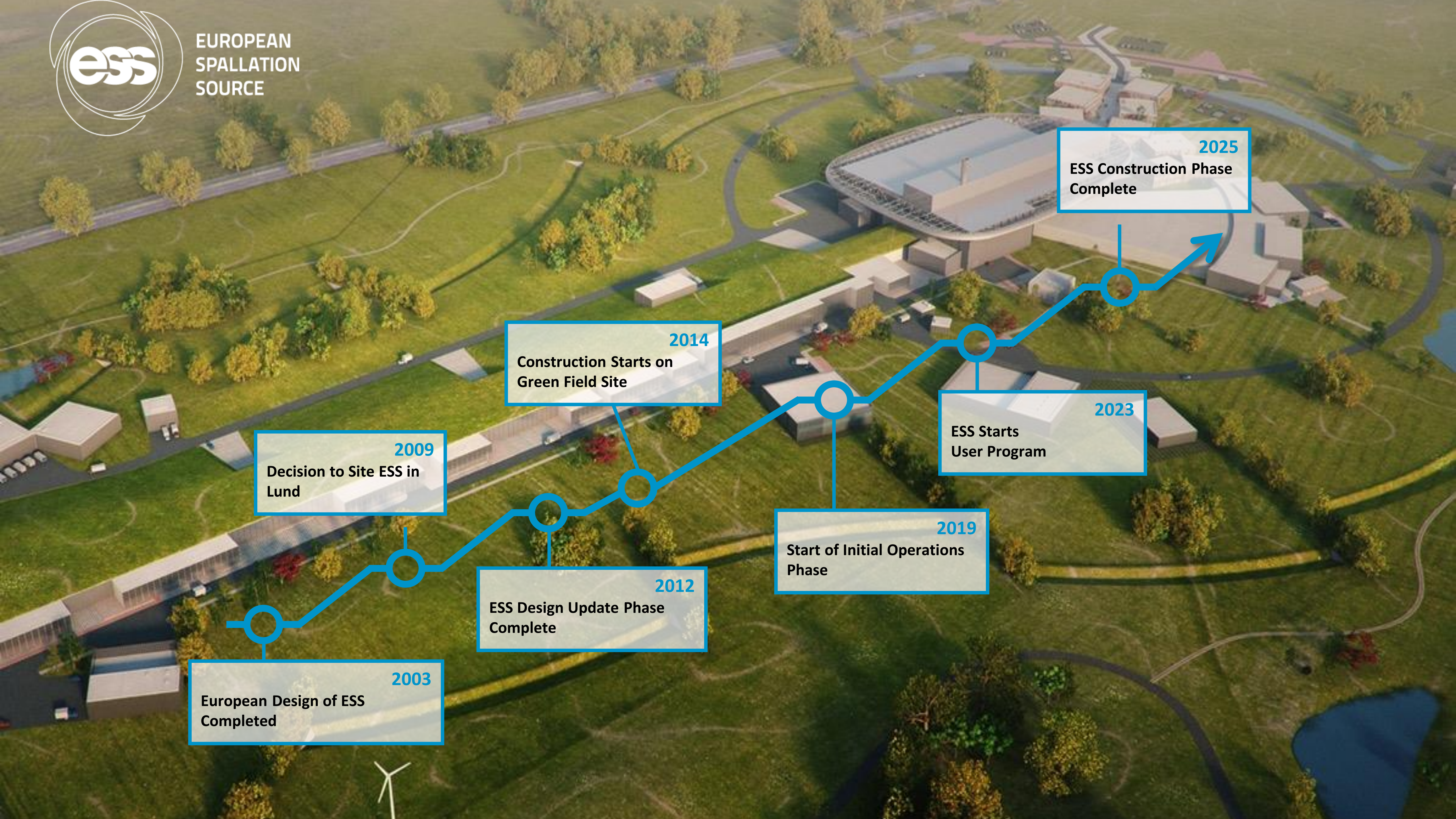
How does ESS compare?



EUROPEAN
SPALLATION
SOURCE

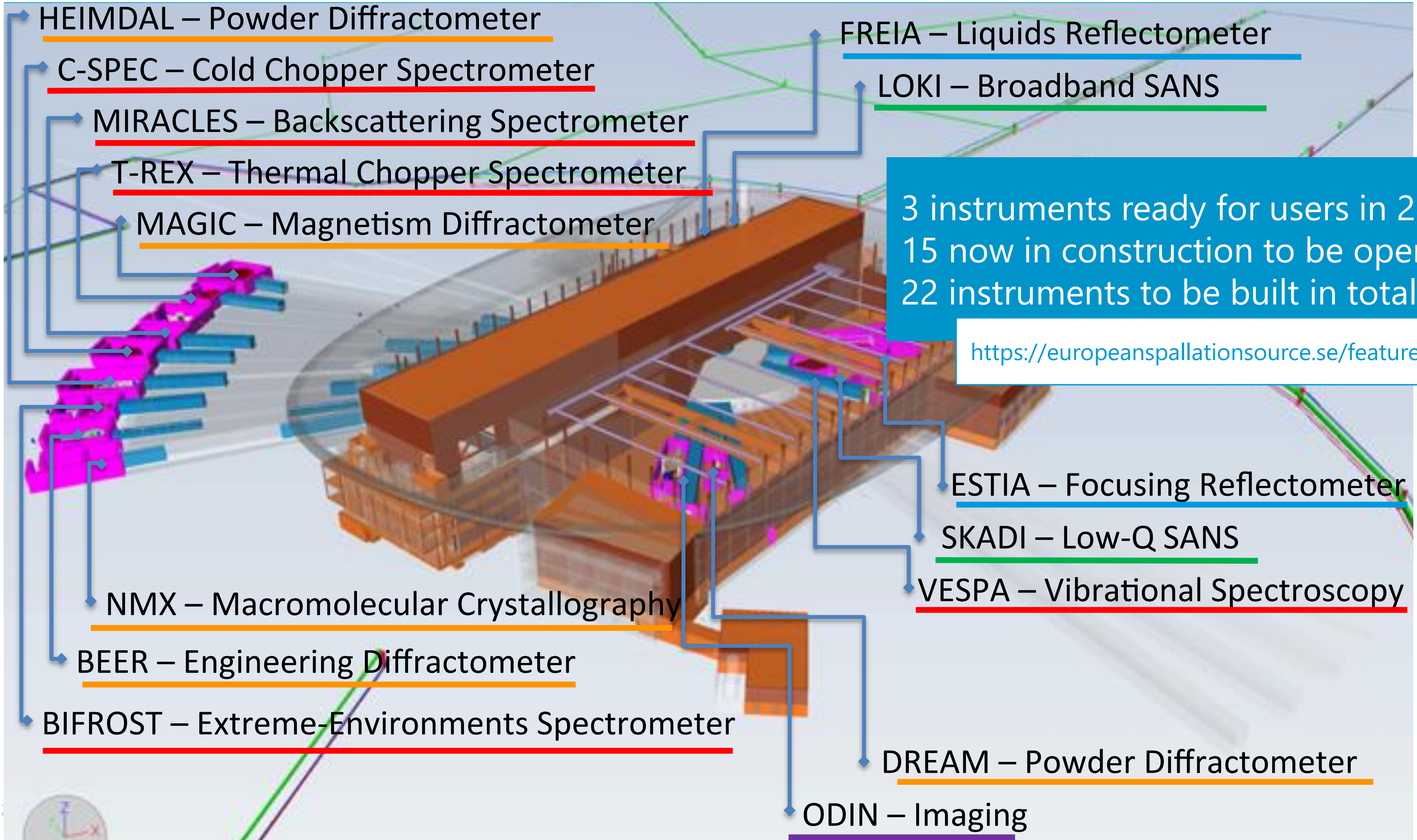
1843 M€	construction cost
5 MW	world's most powerful particle accelerator
2.86 ms	long pulse spallation source
14 Hz	pulse repetition rate
15	instruments in initial suite
2023	first science for users
15	ERIC members and observer nations




EUROPEAN SPALLATION SOURCE
2003
European Design of ESS Completed
2009
Decision to Site ESS in Lund
2012
ESS Design Update Phase Complete
2014
Construction Starts on Green Field Site
2019
Start of Initial Operations Phase
2023
ESS Starts User Program
2025
ESS Construction Phase Complete

Neutron Science Instruments at ESS

1 Imaging, 2 SANS, 2 Reflectometers, 5 Spectrometers, 5 Diffractometers



3 instruments ready for users in 2024
15 now in construction to be operational by 2028
22 instruments to be built in total

https://europeanspallationsource.se/feature-series-ess-instrument-suite

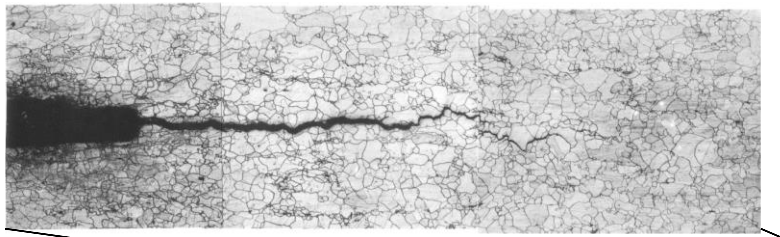
Science with Neutrons

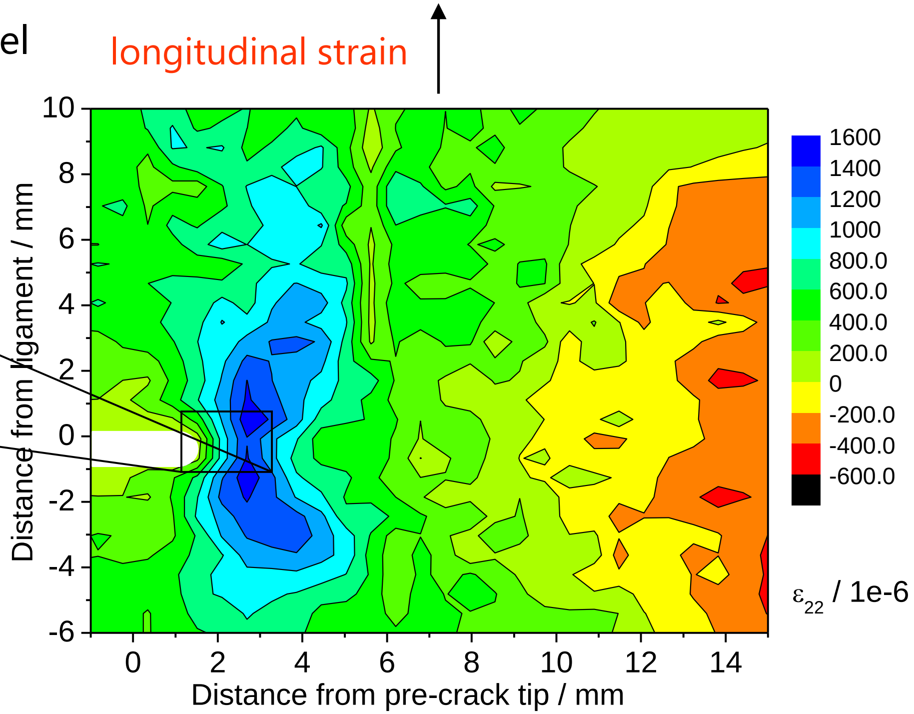
Addressing challenges in energy, materials and health

Neutrons for Materials

Understanding macroscopic behaviour from nanostructure

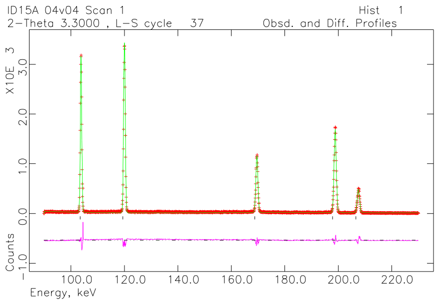
Fatigue + Creep Crack in **25mm** Austenitic steel





Aim: Exploring the boundaries of spatial resolution achievable in real materials engineering components, using combinations of in-situ techniques: imaging & diffraction, in-situ loading, high-temperature…

Methods: Scanning neutron diffraction and time-of-flight imaging



Neutrons for Materials

Mechanical Deformation of Composites

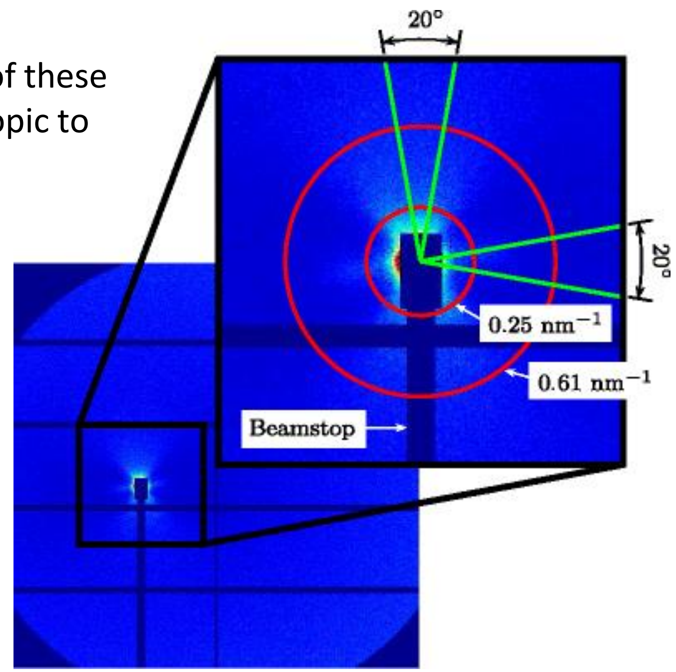
Polymer blends and composites are key materials in modern manufacturing

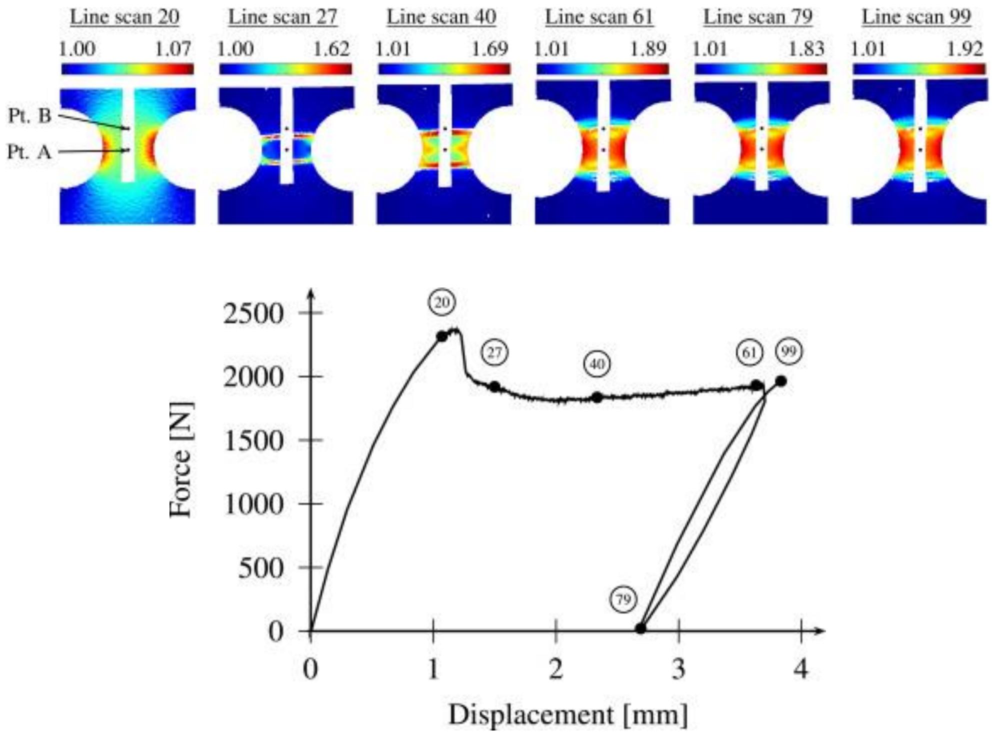
Need to understand the deformation of these materials under strain - from macroscopic to microscopic

Combination of digital image correlation (DIC) and SAXS over a wide Q range

In-situ strain – mechanical, electro-deformation, and magneto-deformation.

Using small beams to scan over sample to get distribution of deformation / structural change





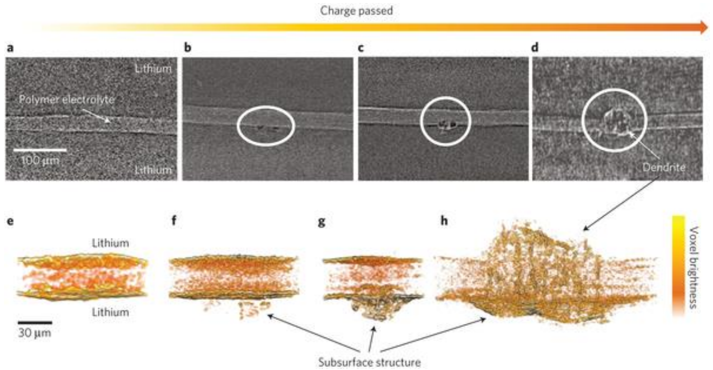
Engqvist et al Polymer, 2016
https://doi.org/10.1016/j.polymer.2015.11.028

Neutrons for Clean Energy Technology

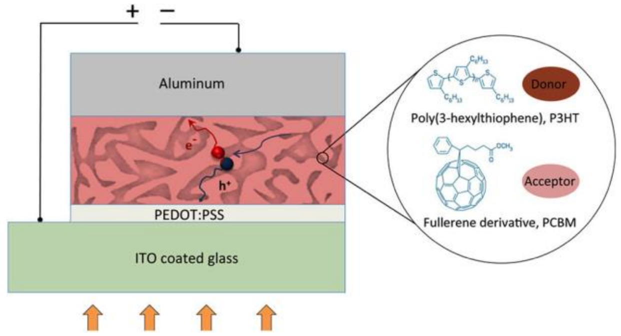
Probing Light Elements

Lithium Ion Batteries are a crucial technology for the expansion of electric vehicle use and for mobile computing.

Analysis of **operating devices** allows the monitoring of **nano- and micro-structural change.**



Dendrite growth in lithium metal anode batteries observed by x-ray microtomography. (Harry et al. (2013) Nature Materials 13, 69)

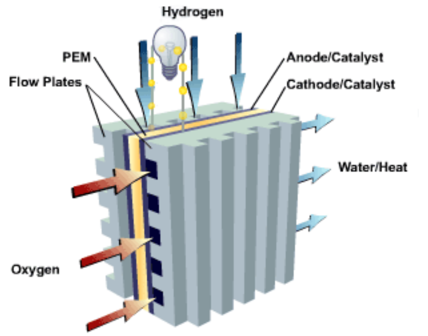


Organic Solar Cells promise to provide cheap and accessible solar energy.

Understanding the **structural evolution** under operation guides development of new devices.

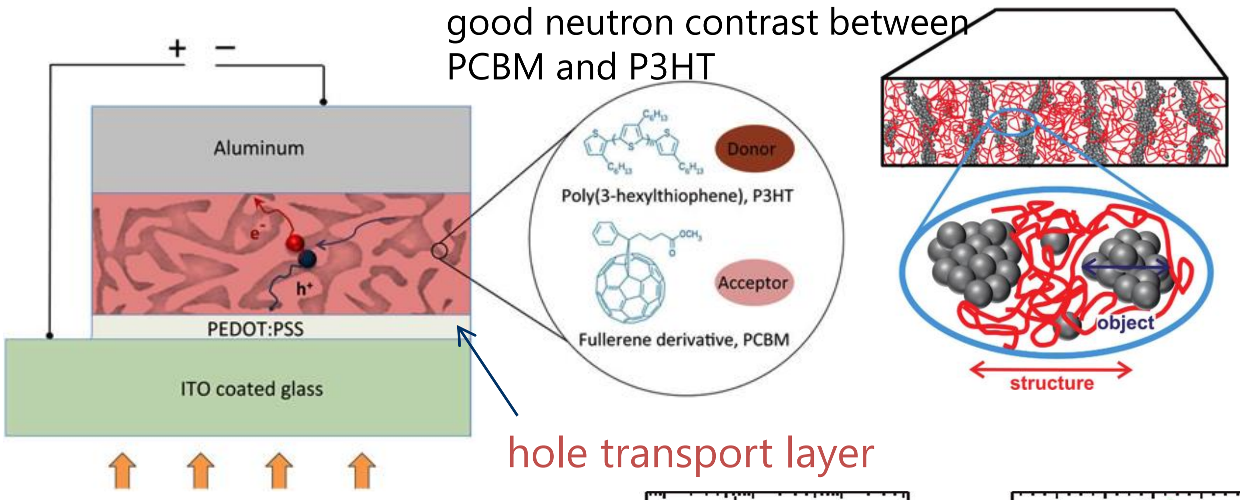
Fuel Cells promise to provide carbon free energy.

Understanding the **details of the ionomer membranes** is key to development of better devices



Neutrons for Clean Energy Technology

Nanostructure in Organic Solar Cells – crystallinity and phase separation

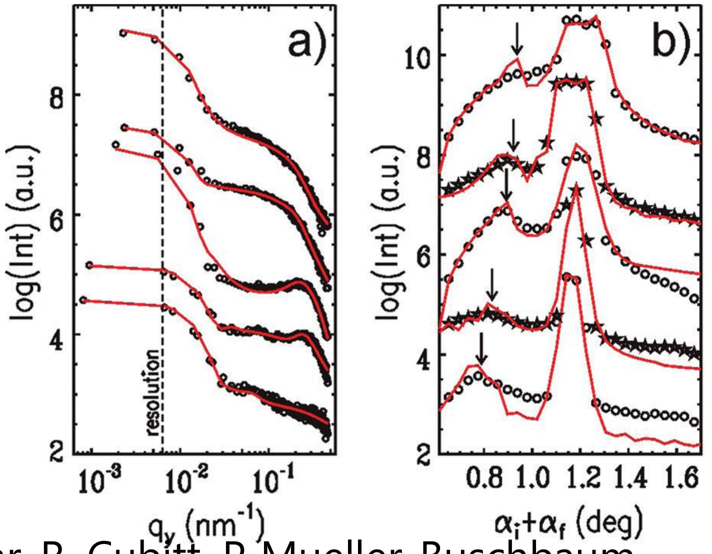


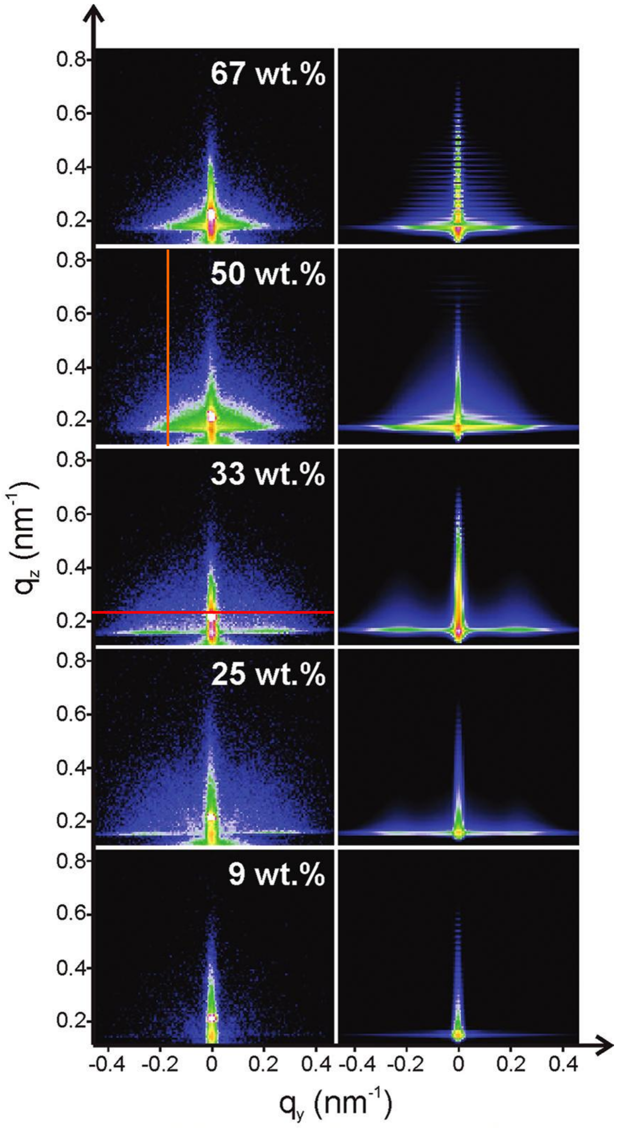
a) GISANS horizontal cuts: particle and domain size

b) GISANS vertical cuts:-> composition of phases

c) GISAXS: -> crystallinity

Increasing molecularly dispersed PCBM with higher content ≠ pure phases

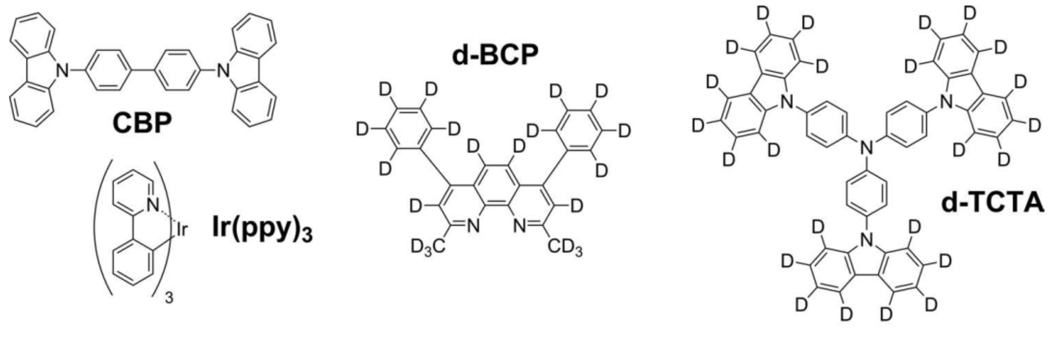


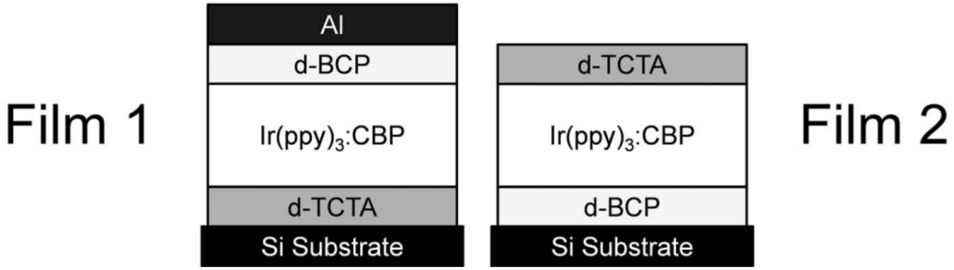


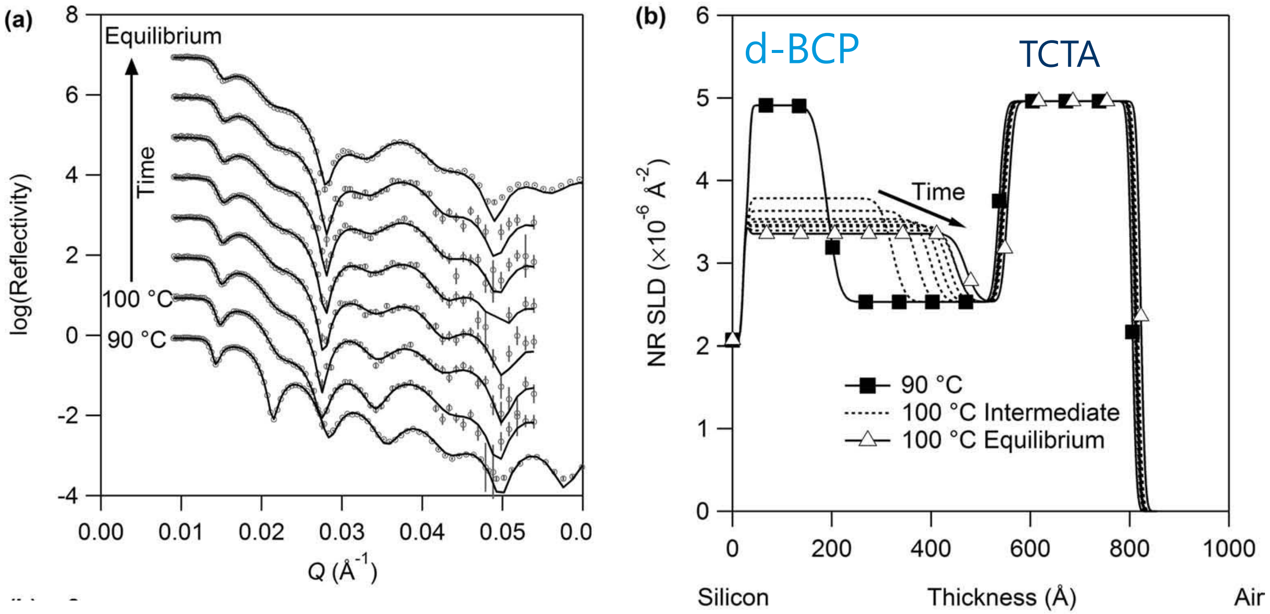
M.A. Ruderer, R. Meier, L. Porcar, R. Cubitt, P. Mueller-Buschbaum, Journal of Physical Chemistry Letters, 3 (2012) 683-688.

Neutrons for Clean Energy Technology

Interdiffusion in OLEDs - Neutron contrast provides chemical information







OLED performance depends on compartmentalization of active layers. Operating temperatures cause interdiffusion and degradation of photoluminescence.

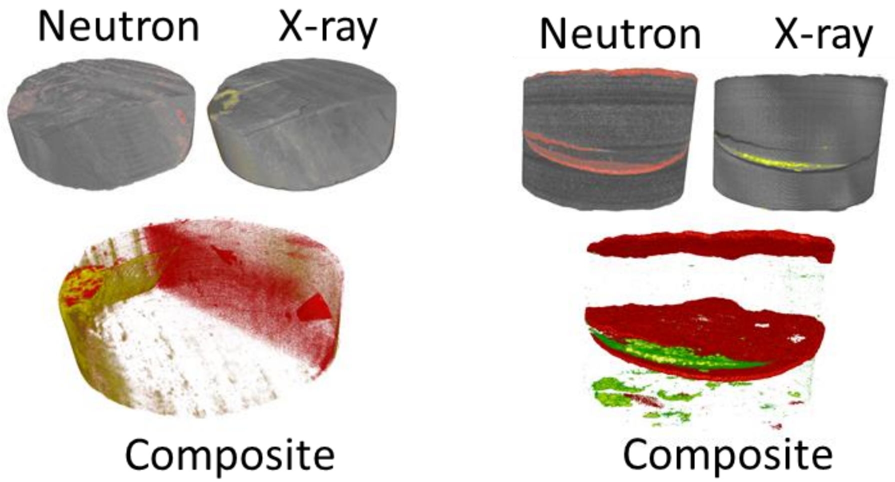
Good neutron contrast by deuterium labeling of TCTA and BCP allows determination of vertical concentration profile.

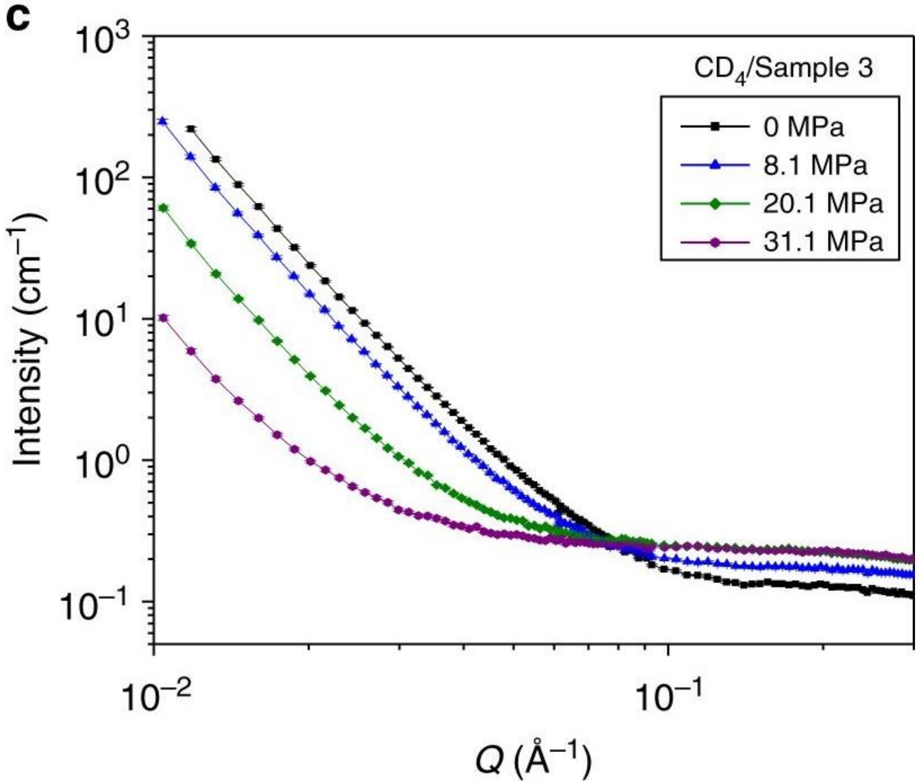
A.R.G. Smith et. al. , Advanced Materials, 24 (2012) 822-826.

Neutrons for Oil and Gas Exploration

Shale Gas Deposits

- Need correlations of organic matter to shale structure
- SANS for pore size distribution, chemistry
- Neutron and X-ray tomography (NeXT) provides macroscopic map



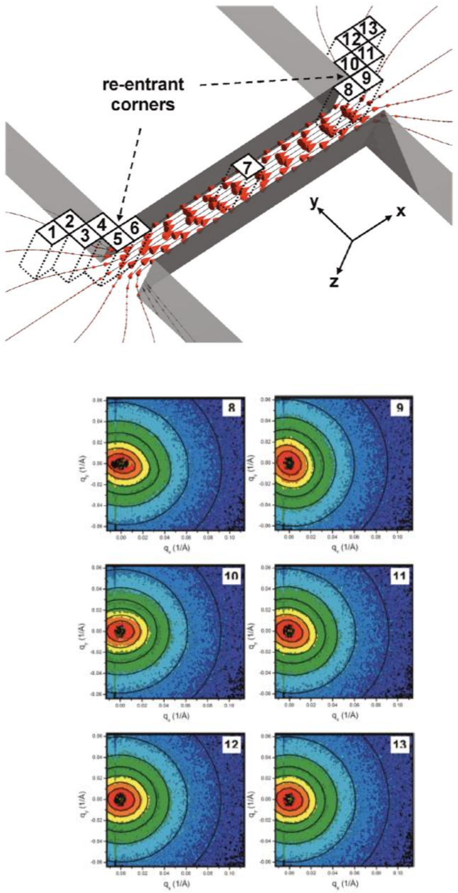


W. S. Chiang, E. Fratini, P. Baglioni, D. Georgi, J. Chen, Y. Liu *J. Phys. Chem. C* ***120****, 4354 (2016)*
W. S. Chiang, E. Fratini, P. Baglioni, D. Georgi, J. Chen, Y. Liu *Langmuir* **32**, 8849 (2016)
W.-S. Chiang, J. M. LaManna, D. S. Hussey, D. L. Jacboson, Y. Liu, J. Zhang, D. T. Georgi, J. R. Kone, J.-H. Chen, *Petrophys.* **59**, 153 (2018)
W. S. Chiang, D. Georgi, T. Yildirim, J. Chen, Y. Liu *Nature Communications* **9**, 784 (2018)

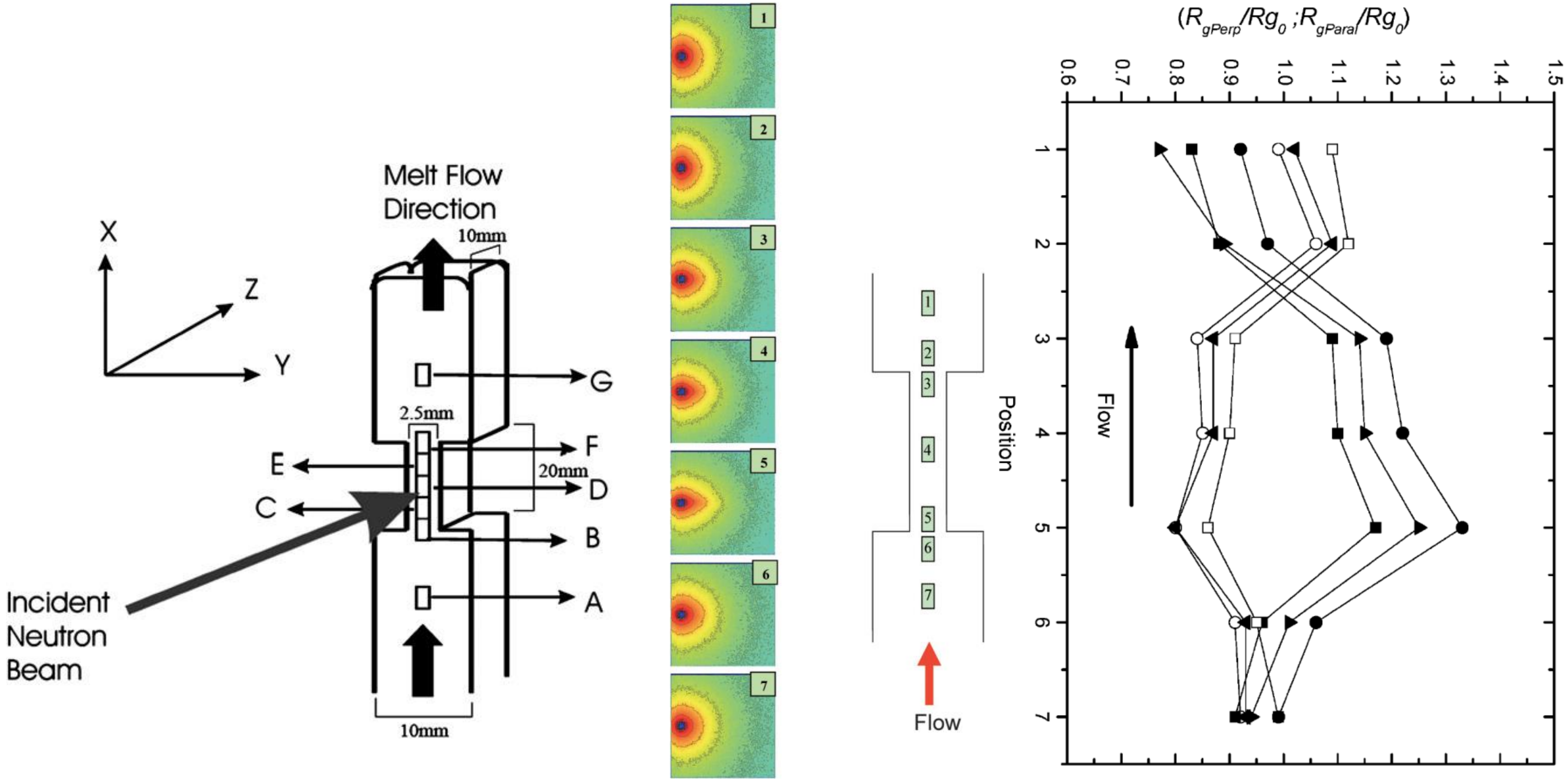
Neutrons for Plastics and Polymers

Polymer Flow

Measuring the deformation of polymer chains allowing development of new models of polymer flow



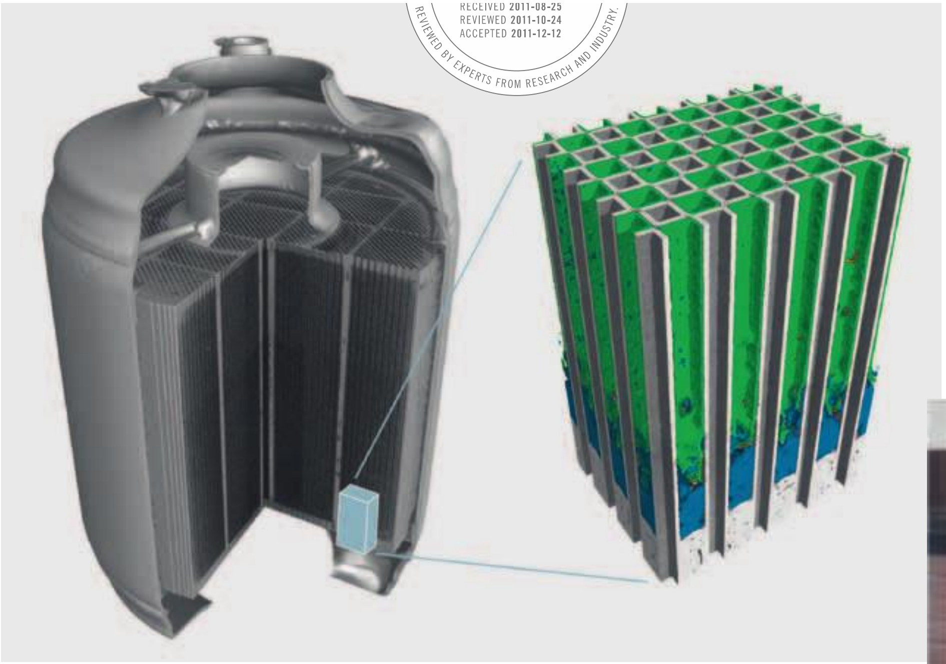
Clarke et al. (2010) Macromolecules 43, 1539



McLeish et al., *Soft Matter*, 2009, **5**, 4426

Neutrons for Industrial Equipment

Visualising Particle Distributions - chemical sensitivity gives enhanced information

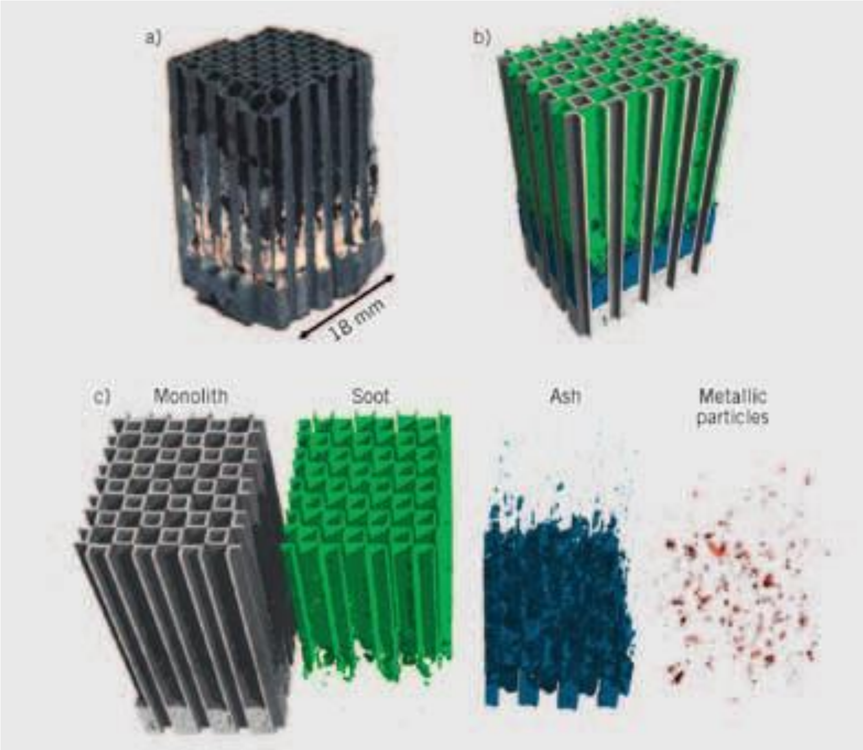


AUTHORS

DR. DIPL.-PHYS.
CHRISTIAN GRÜNZWEIG

VISUALISING THE SOOT AND ASH DISTRIBUTION IN DIESEL PARTICULATE FILTERS USING NEUTRON IMAGING

Neutron tomography is presently the only possibility to obtain information about



Neutron tomography used to examine particulate type and distribution in filters

The chemical sensitivity of neutrons allows identification of the particle types

Courtesy: Ch. Gruenzweig, PSI, Switzerland

Neutrons for Agriculture & Food

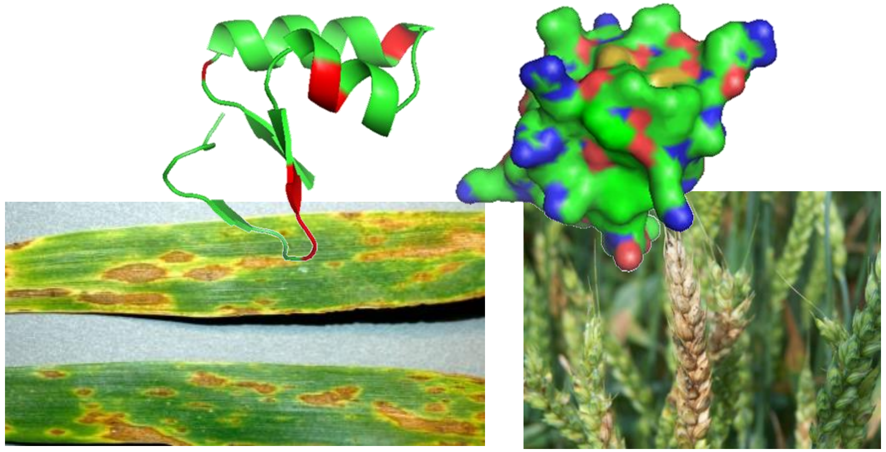
Antimicrobial & Antifungal Proteins in Plants

α-purothioins

(A)

$α_1$-Pth	KSCCRSTLGR NCYNLCRARG AQKLCAGVCR CKISSGLSCP KGFPK
$α_2$-Pth	KSCCRTTLGR NCYNLCRSRG AQKLCSTVCR CKLTSGLSCP KGFPK

(B) (C)



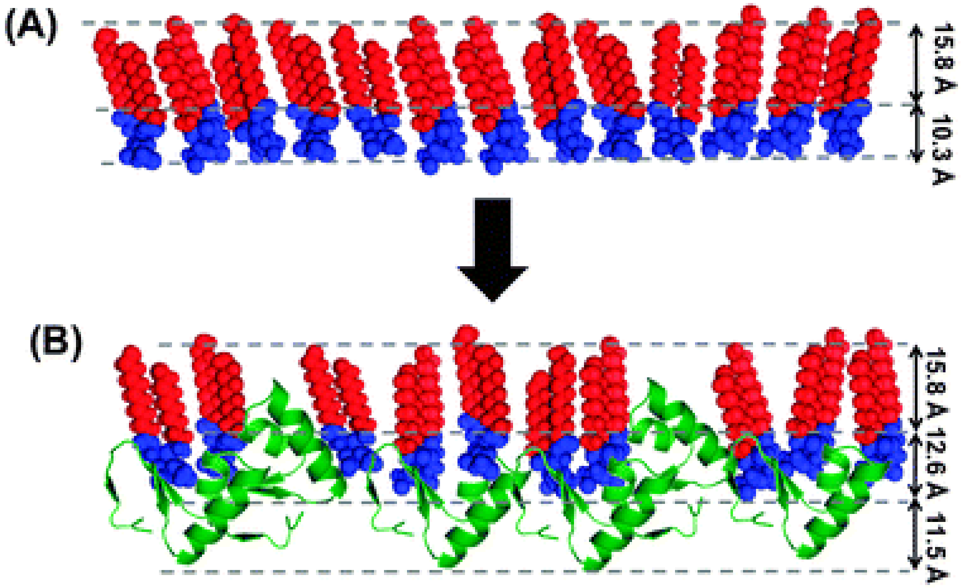
Tan spot (*Pyrenophora tritici-repentis*)

Glumbe Blotch (*Stagonospora nodorum)*

Common Smudge (*Cochliobolus sativus)*

Stripe blight (*Pseudomonas syringie)*

Neutron reflectometry used to determine how plant defence proteins from common wheat interact with cell membranes.

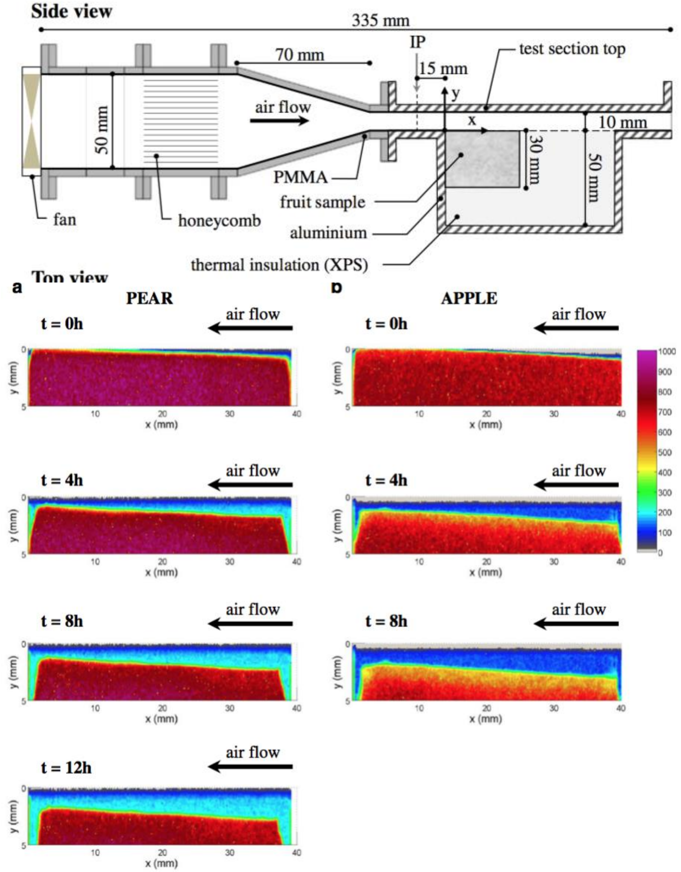


Clifton et al. *Phys. Chem. Chem. Phys.*, 2012, 14, 13569-13579

Neutrons for Agriculture & Food

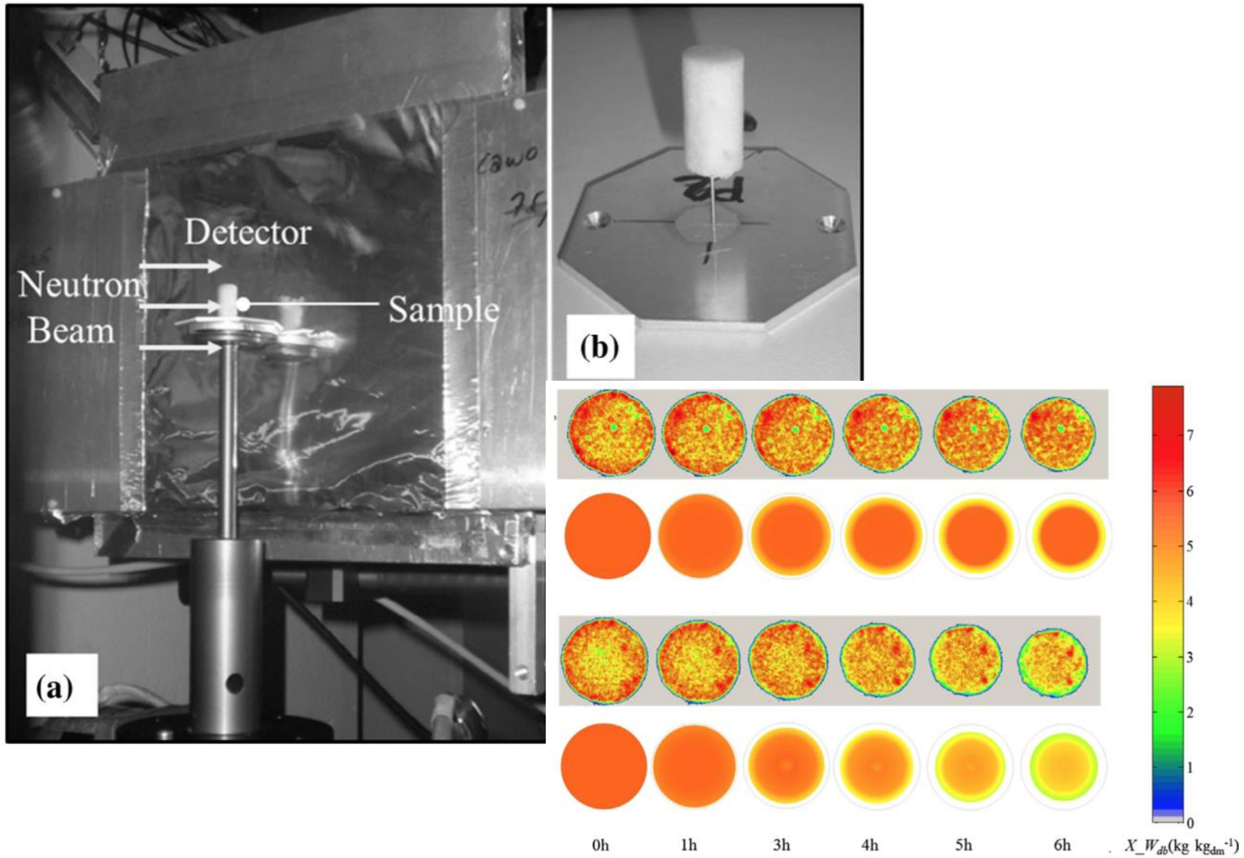
Drying of Fruit

In-Situ drying in wind tunnel using neutron imaging to quantitatively determine water loss and water loss profile



Defraeye, T., et al. *Food and Bioprocess Technology*, *6*(12), 3353

Neutron tomography of dehydration of apple used to examine water loss and validate numerical simulations of drying



Aregawi, W., et al. (2013). *International Journal of Heat and Mass Transfer* , *67*, 173–182.

Neutrons for Clean Water

Understanding Natural Flocculants

- Removal of contaminant particles is a key first step in water purification.
- Chemical flocculants are expensive and potentially harmful if released
- The use seed pulp from Moringa oleifera trees has been used to clarify water
- Optimising this by finding and using the specific proteins that do the flocculation can provide a low cost, natural solution for water purification.
- (U)SANS and SAXS to find structure and concentration of flocs
- Neutron and X-ray tomography (NeXT) provides macroscopic map

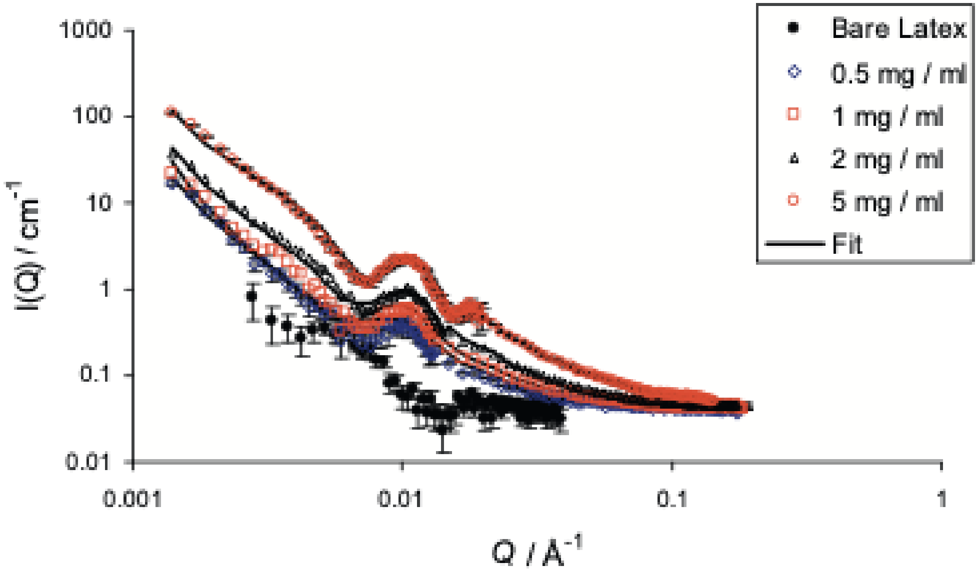
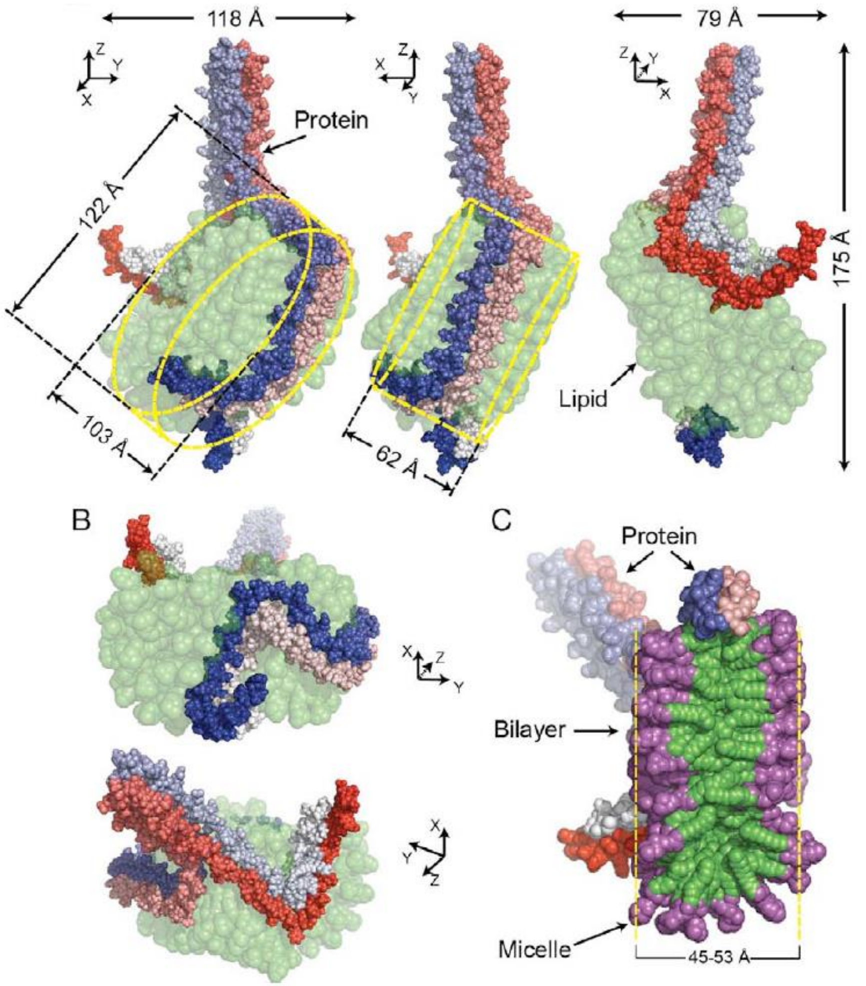


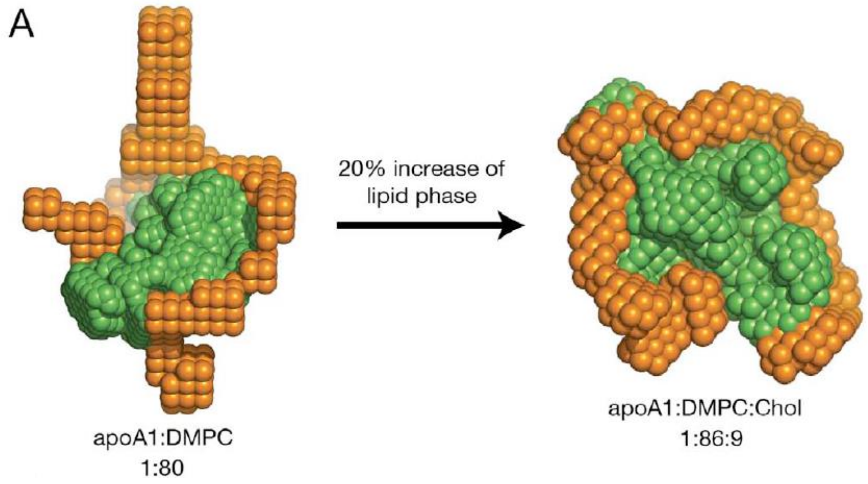
Fig. 2. Small-angle scattering from the deuterated latex in D_2O with added *Moringa oleifera* protein. The samples with different protein concentrations are shown with fits to a core–shell model with residual protein that accounts for the adsorbed layer.

M.S. Hellsing, et al., Structure of flocs of latex particles formed by addition of protein from Moringa seeds, Colloids Surf. A: Physicochem. Eng. Aspects (2013), http://dx.doi.org/10.1016/j.colsurfa.2013.11.038

Neutrons for Biotech and Medicine

Structure of High Density Lipoprotein in Solution





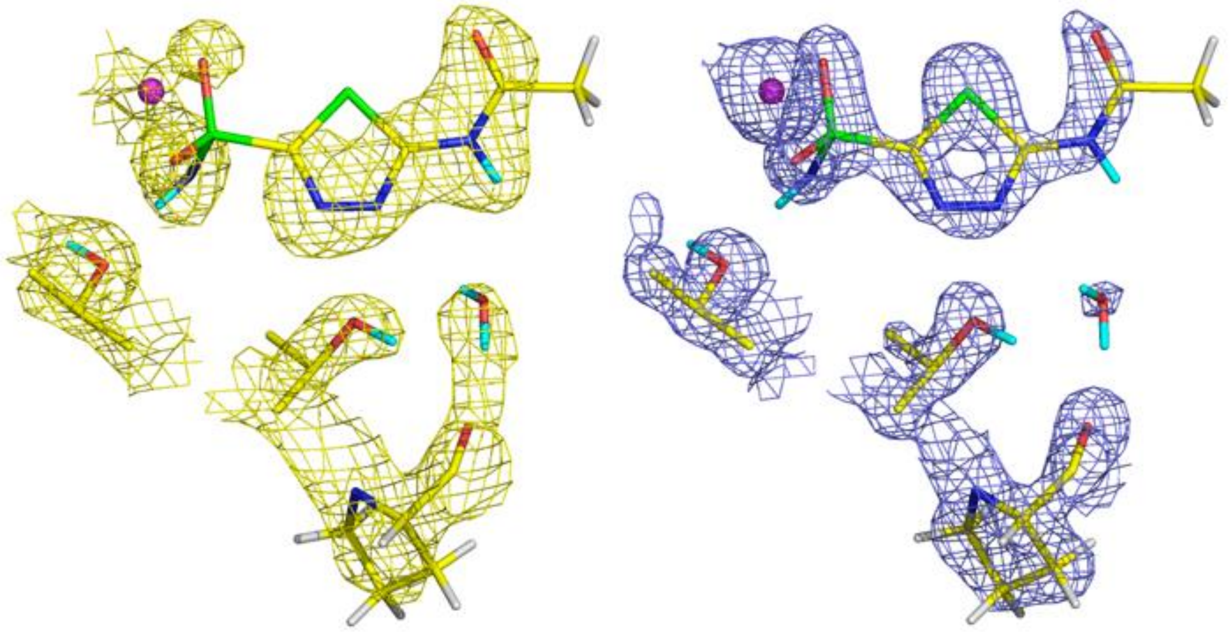
Small Angle Neutron Scattering used to determine the low resolution structure of nascent high density lipoprotein with and without cholesterol.
This reveals a mechanism for particle expansion

V. Gogonea et al., Journal of Lipid Research, (2013).

Neutrons for Biotech and Medicine

Drug-Target Binding

Macromolecular crystallography: “go to” technique for rational drug design.
X-rays and neutrons combined can elucidate specific binding interactions between drug and disease target.
Data can reveal protonation state of ligands.
Can determine the atomic details of drug binding as mediated by hydrogen bonding, solvent-mediated interactions, and which groups of the protein and/or drug are directly involved.
** Get clues about which parts of the drug to target for modification.



Clinically used drug (acetazolamide) in complex with human drug target, carbonic anhydrase.

Yellow: nuclear density maps reveal H atoms

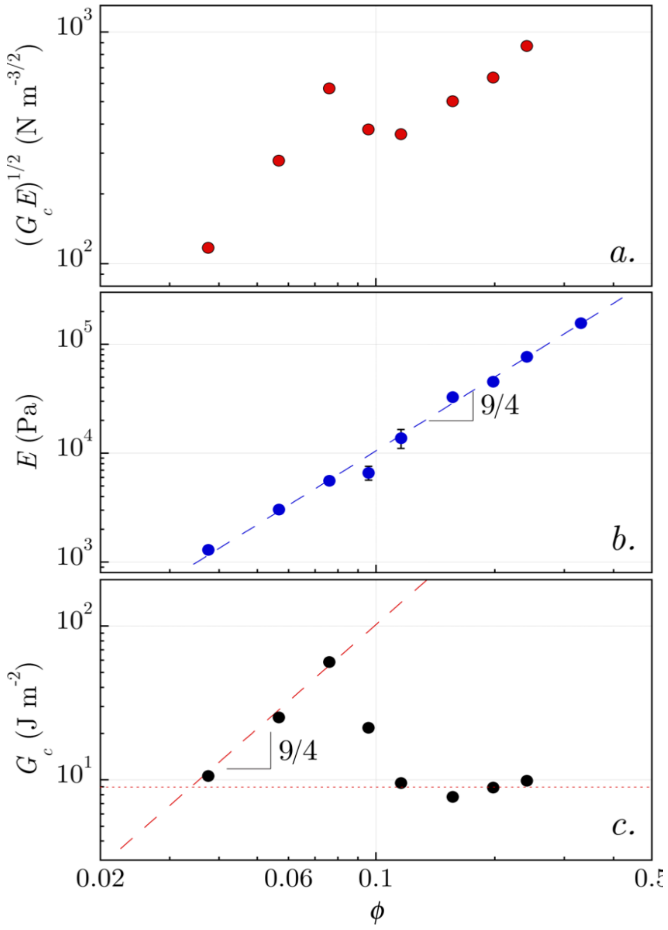
Blue: electron density maps reveal positions of heavier atoms

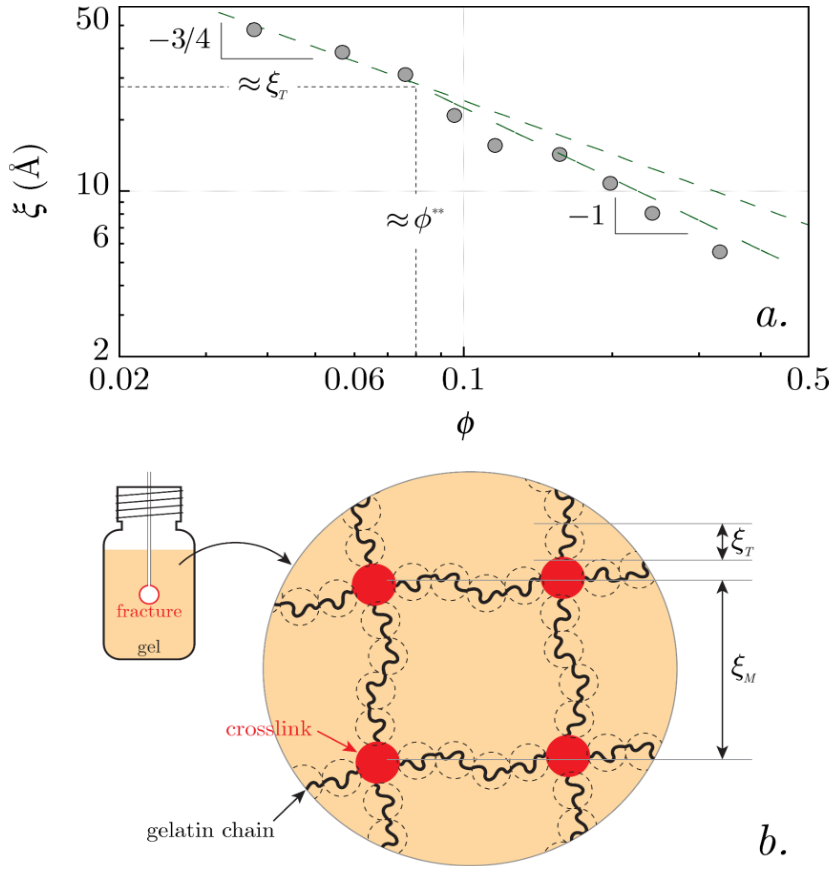
Joint X-ray & neutron studies reveal the “full” details of drug binding (water-mediated, H-bonds). Complementary!
Fisher et al. (2012) JACS 134, p.14726.

Neutrons for Biotech and Medicine

Gelatin Fracture Mechanisms

- Soft gel products are critical to OTC drug formulations
- Performance varies across globe
- SANS and poroelasticity measurements provide molecular insight into burst time
- New formulations being tested for adoption





B. R. Frieberg R.-S. Garatsa R. L. Jones, J. O. Bachert, III B. Crawshaw, X. M. Liu and E. P. Chan, *Soft Matter* ***14****, 4696 (2018)*

Summary

Why you should start using neutrons …

Neutrons are a non-destructive, penetrating probe of structure on the atomic to macroscopic scale.

Neutrons provide chemical sensitivity being especially sensitive to light elements.

Neutron scattering can be isoptope dependent, so contrast variation using H/D substitution allows complex structures to be more easily understood

Thank you! Any Questions?

Want to know more?

Website : **http://www.europeanspallationsource.se**

Contact me : **andrew.jackson@ess.eu**

Materials from Sweden Podcast Episode about ESS and neutrons :

https://www.podbean.com/ew/dir-ef4kx-6448f66