

# Fundamental Research with Neutrons

Andrew Jackson

European Spallation Source

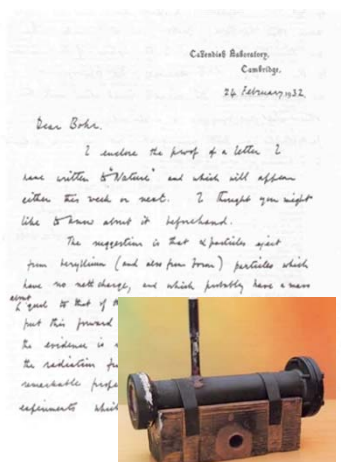
Delivered by Wim Bouwman, Delft University of Technology

75 years of nuclear reactors: A chain reaction of applications  
KIVI-NNS Symposium, 3rd November 2017

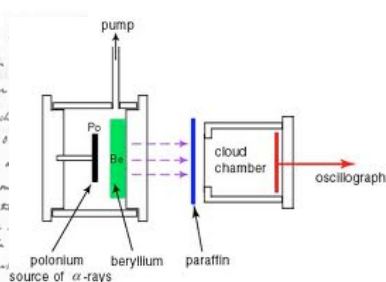
## The Neutron

1932 Discovery of the neutron by Chadwick (prediction by Rutherford 1920)

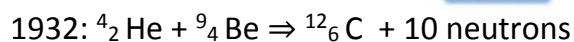
“Whatever the radiation from Be may be,  
it has most remarkable properties”



letter to 'Nature' and they can all intelligently readily on the assumption the particles are neutrons. Further taken some pictures in the separation cell and we have already found about 20 of these atoms. About 4 of these show a head (and it is almost certain that 100% of the fork represents a neutral atom and the same other particles, probably an  $\alpha$  particle, are disintegrated due to the capture of the by  $N_2$  or  $O_2$ . I enclose two photographs one of which shows the simple neutral atom, and other what we suppose is a disintegration. The photographs are not very good but they were presented in a hurry.



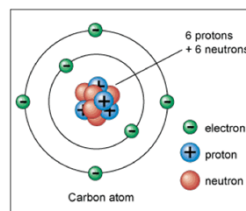
With best regards  
Yours sincerely  
J. Chadwick.



## The Neutron

The neutron:

- Is a spin 1/2 sub-atomic particle
- Has a mass equivalent to 1839 electrons ( $1.674928 \times 10^{-27}$  kg or 939.57 MeV)
- Has a magnetic moment of  $-1.9130427 \mu_n$  ( $-9.6491783 \times 10^{27}$  JT<sup>-1</sup>)
- Has a lifetime of 15 minutes (885.9 s).



Neutrons are baryons  
Three quarks (udd) = neutron



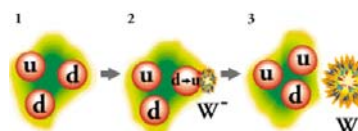
### Waveparticle duality

Particle and a Wave

- Reflection
- Diffraction
- Refraction
- Focussing

Neutron decays into proton + electron + antineutrino (of the electron type)

$$n \rightarrow p^+ e^- \bar{\nu}_e$$



## Why Neutrons for Research?

**The Nobel Prize in Physics 1994**

**Neutrons reveal structure and dynamics**

**S Clifford G. Shull, MIT, Cambridge, Massachusetts, USA, receives one half of the 1994 Nobel Prize in Physics for development of the neutron diffraction technique.**

**B Bertram N. Brockhouse, McMaster University, Hamilton, Ontario, Canada, receives one half of the 1994 Nobel Prize in Physics for the development of neutron spectroscopy.**

Neutrons show where atoms are

Neutrons show what atoms do

Neutrons bounce against atomic nuclei. They also react to the magnetism of the atoms.

Neutrons are unique as particles and as waves.

The Royal Swedish Academy of Sciences has awarded the 1994 Nobel Prize in Physics for pioneering contributions to the development of neutron scattering techniques for studies of condensed matter.

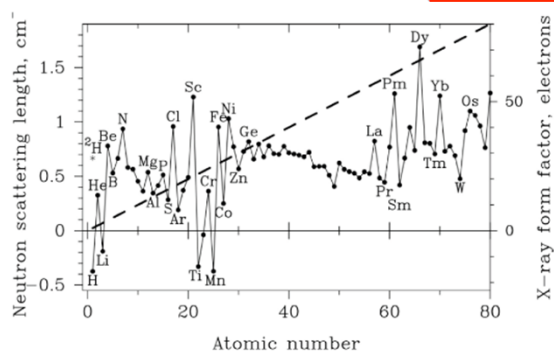
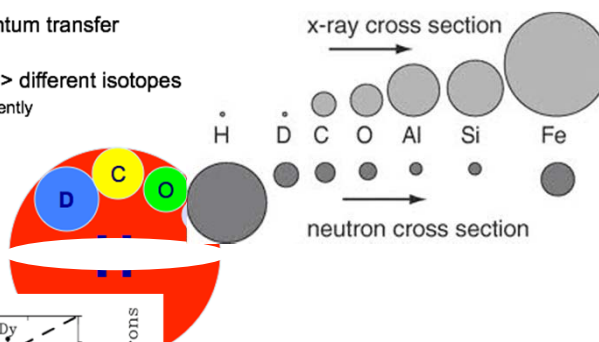
With his 3-axis spectrometer Brockhouse measured energies of phonons (atomic vibrations) and magnons (magnetic waves). He also studied how atomic structures in liquids change with time.

Because of the wave nature of neutrons, a diffraction pattern can be recorded which indicates where in the sample the atoms are situated. Even the placing of light elements such as hydrogen in metallic hydrides, or hydrogen, carbon and oxygen in organic substances can be determined.

The pattern also shows how atomic dipoles are oriented in magnetic materials, since neutrons are affected by magnetic forces. Shull also made use of this phenomenon in his neutron diffraction technique.

## Why Neutrons for Research?

- 1) Ability to measure both energy *and* momentum transfer  
Geometry of motion
- 2) Neutrons scatter by a nuclear interaction => different isotopes scatter differently  
H and D scatter very differently
- 3) Simplicity of the interaction allows easy interpretation of intensities  
Easy to compare with theory and models
- 4) Neutrons have a magnetic moment



$$V(r) = \frac{h^2}{2\pi m} \left\langle \sum_i b_i \delta(\mathbf{R} - \mathbf{r}_i) \right\rangle$$

Interaction of neutron and nucleus is described by the pseudo-potential developed by Fermi

## Contrast matching to make parts structure (in)visible



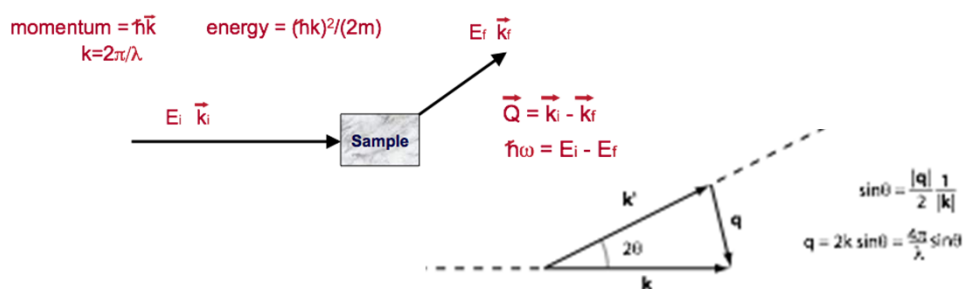
Morna Fisker, Brillab  
<https://youtu.be/CZxwlc3ieM>

## Many materials transparent for neutrons In situ during processing



Anders Kaestner, PSI  
<https://youtu.be/VESMU7JfVHU>

## What do we measure?

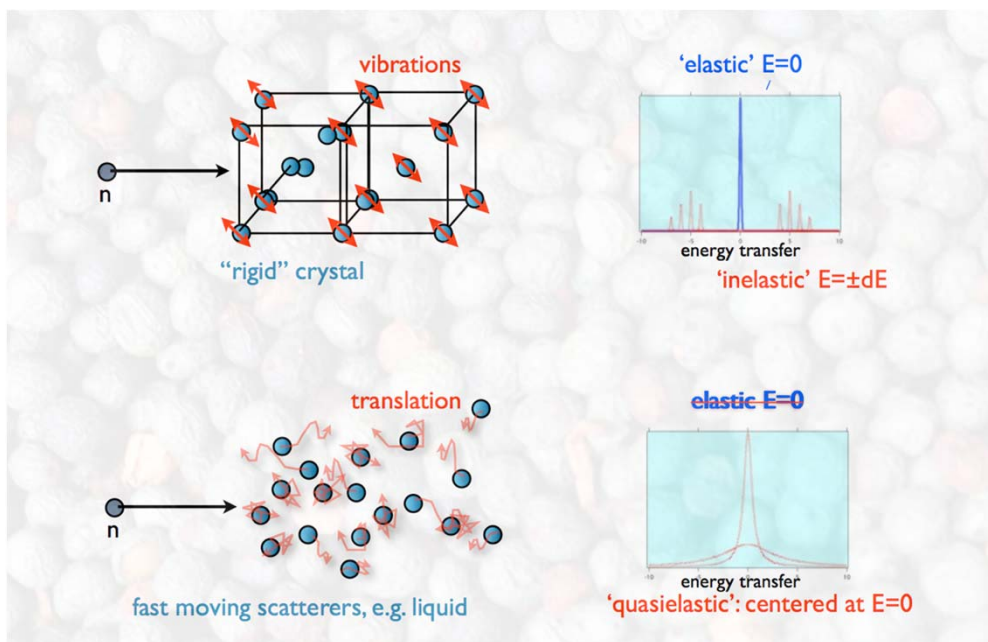


Measure number of neutrons scattered as function of  $Q$  and  $\omega$

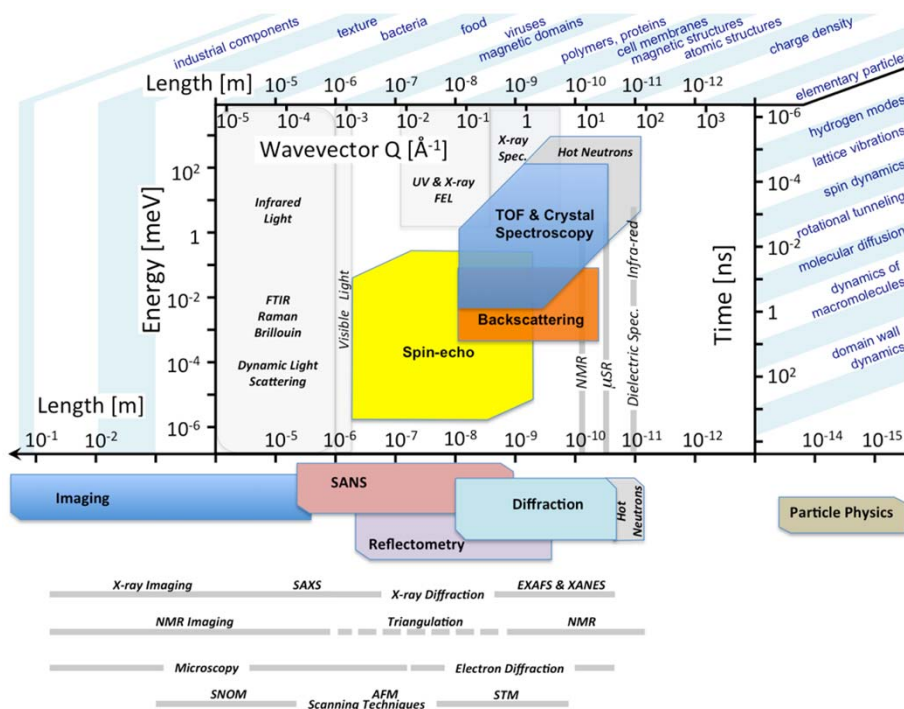
Intensity of scattering as function of  $Q$  is related to the Fourier transform of the spatial arrangement of matter in the sample => Correlations in Space

Intensity of scattering as function of  $\omega$  is related to the Fourier transform of the temporal arrangement of matter in the sample => Correlations in Time

### Elastic vs Inelastic

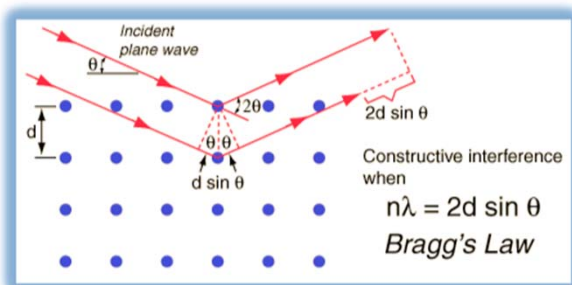


### Neutron Scattering Techniques



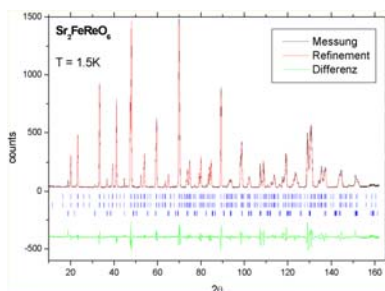
## Diffraction

Sizes probed = "atomic structures" = 0.1 nm - 10 nm



BT1 Diffractometer at NCNR

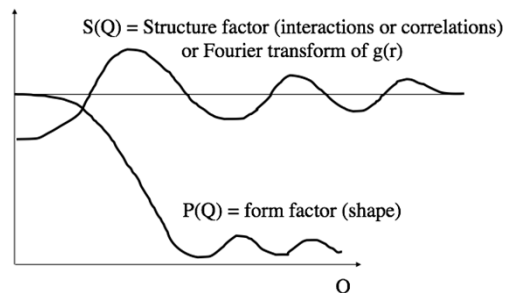
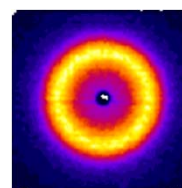
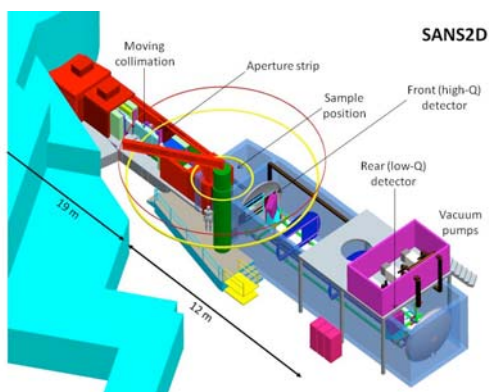
Position and intensity of diffraction peaks gives atomic positions



Diffraction pattern image from [http://www.uni-mainz.de/FB/Physik/IPH/Forschungsbericht02/KOMETexKOMET\\_330\\_NeutronDiffraction.html](http://www.uni-mainz.de/FB/Physik/IPH/Forschungsbericht02/KOMETexKOMET_330_NeutronDiffraction.html)

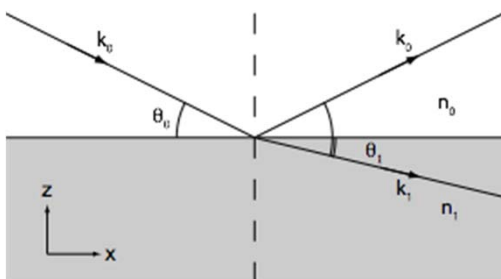
## Small Angle Scattering

Sizes probed = "large-scale structures" = 1 nm - 10  $\mu$ m



## Reflectometry

Sizes probed = 1 nm - 100 nm



NG7 Reflectometer at NCNR

$$k_z = k_0 \sin \theta_0$$

$$q_z = 2k_z = 4\pi/\lambda \cdot \sin \theta_0$$

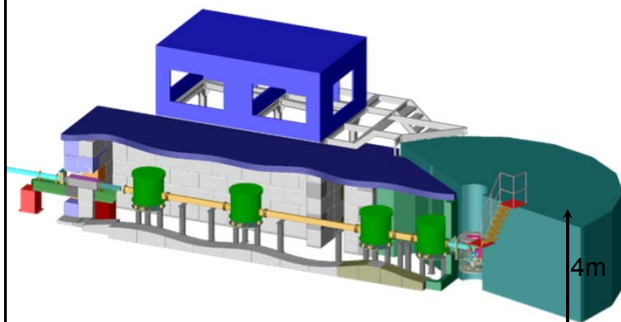
Specular = Incident and Reflected Angles Equal => Structure perpendicular to surface

Offspecular = Incident and Reflected Angles Not Equal => Structure in plane of surface

Reflection of neutrons first shown by Fermi and Zinn in the mid 1940's

## Neutron Spectroscopy

Example : TOFTOF @ FRMII



Measure the change in energy of neutrons as a function of Q to obtain information about atomic or molecular motions

Methods include:

- Triple-axis spectrometry
- Backscattering spectroscopy
- Time-of-flight spectroscopy
- Neutron Spin Echo spectroscopy



Time and spatial resolution are well matched

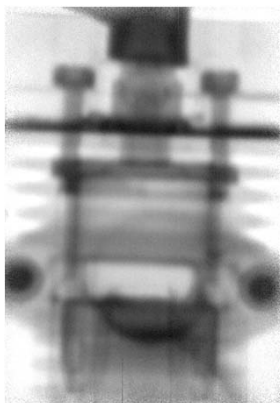
Useful for investigation of diffusive versus confined motion

## Imaging

Mainly radiographic technique

Sizes probed = 100  $\mu\text{m}$  and larger

New methods are developing that give spatial mapping of diffraction or small angle scattering signals

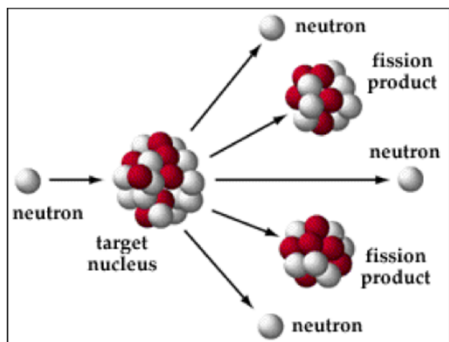


## Neutron Scattering Facilities

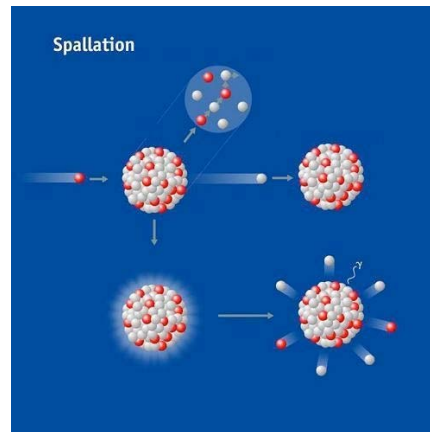


## Types of Neutron Source

### Nuclear Fission (Reactors)



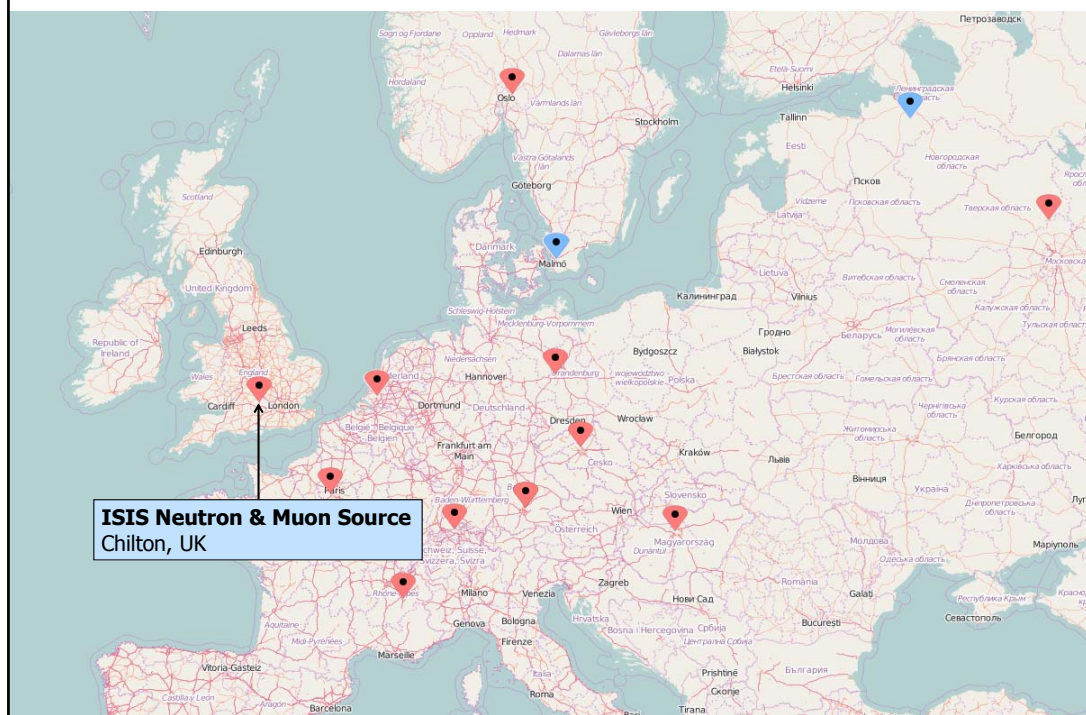
### Spallation



## Neutron Scattering Facilities



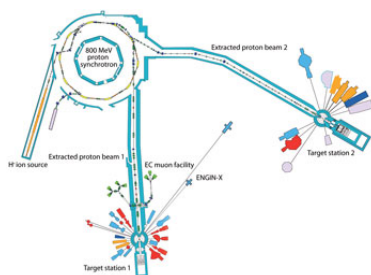
## Neutron Scattering Facilities in Europe



## ISIS Neutron and Muon Source Chilton, UK



- Short pulse spallation source
- Operating since 1984
- Linac and synchrotron ring
- 800 MeV proton beam
- 50 Hz operation
- Tungsten targets
- Hydrogen, Water and Methane moderators
- Two target stations:
  - TS1 – 4/5 pulses (50hz) 160 kW
  - TS2 – 1/5 pulses (10hz) 40 kW
- Recent major upgrade with TS2
- 27 Instruments with 4 in construction
- 1400 users in 3000 visits per year



<http://www.isis.stfc.ac.uk>

## Neutron Scattering Facilities in Europe

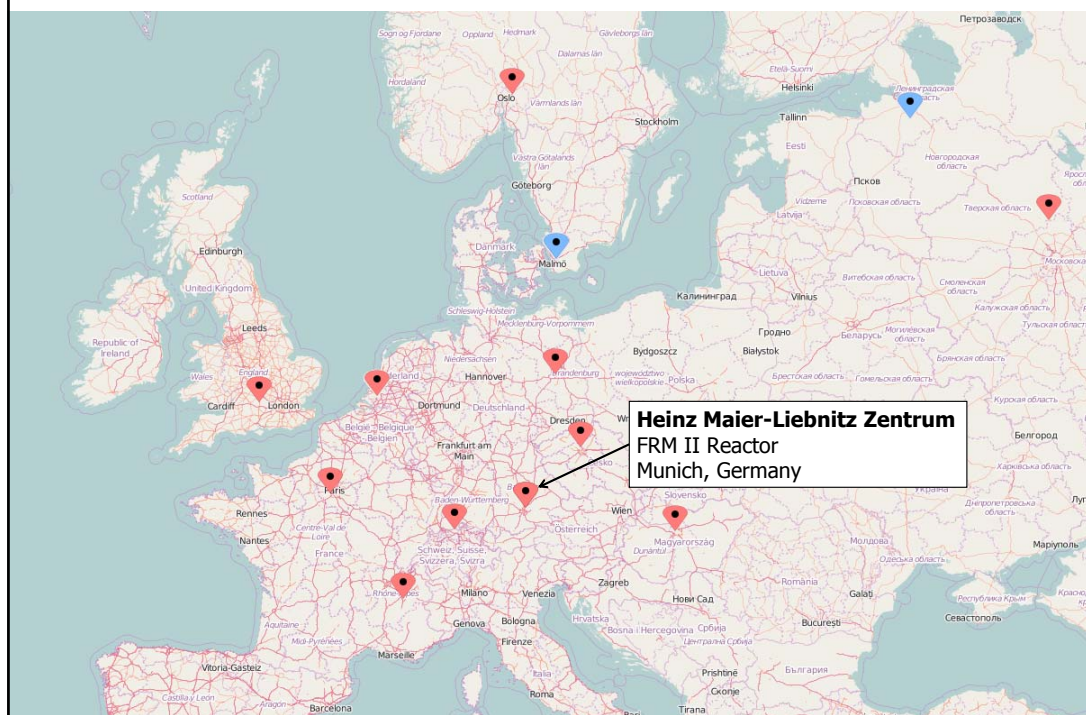


## Institut Laue-Langevin – ILL Grenoble, France





## Neutron Scattering Facilities in Europe



### Heinz Maier-Leibnitz Zentrum – MLZ Munich, Germany

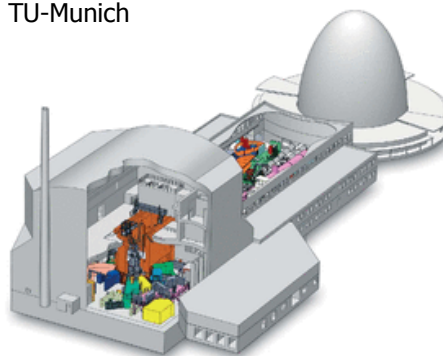
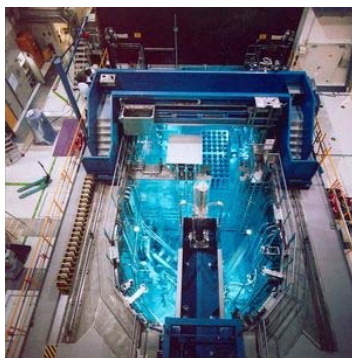


**Helmholtz-Zentrum  
Geesthacht**  
Zentrum für Material- und Küstenforschung

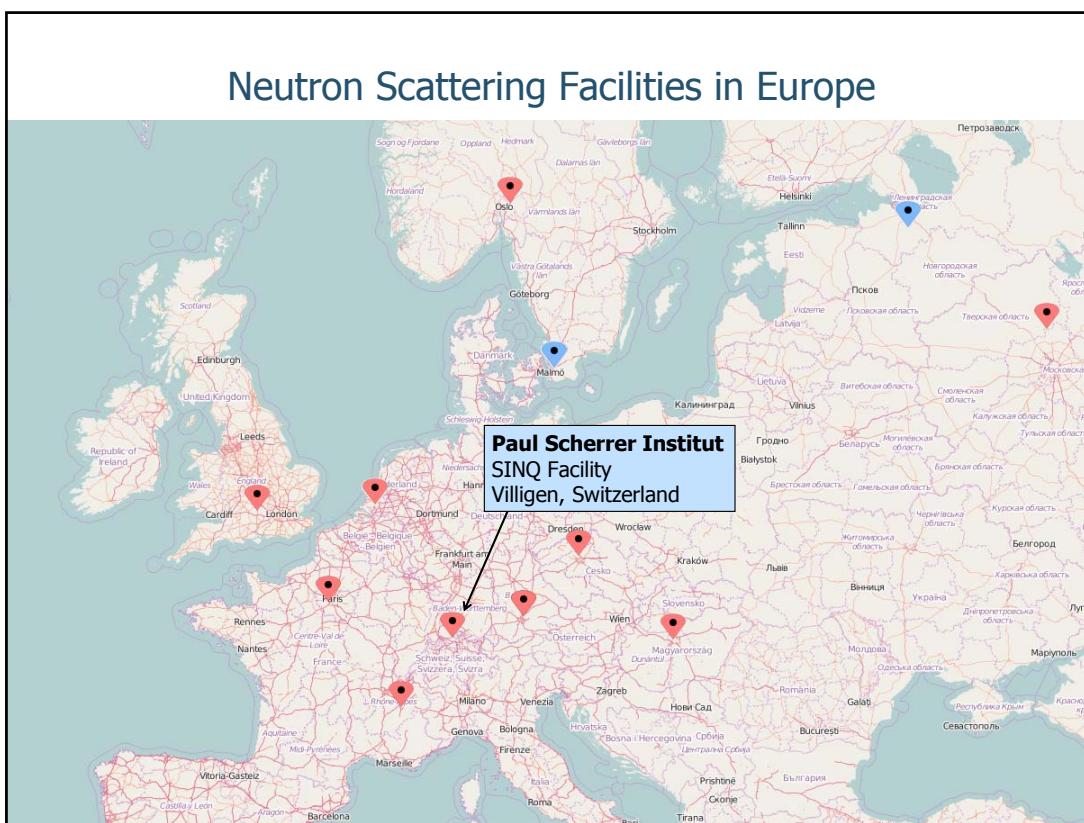
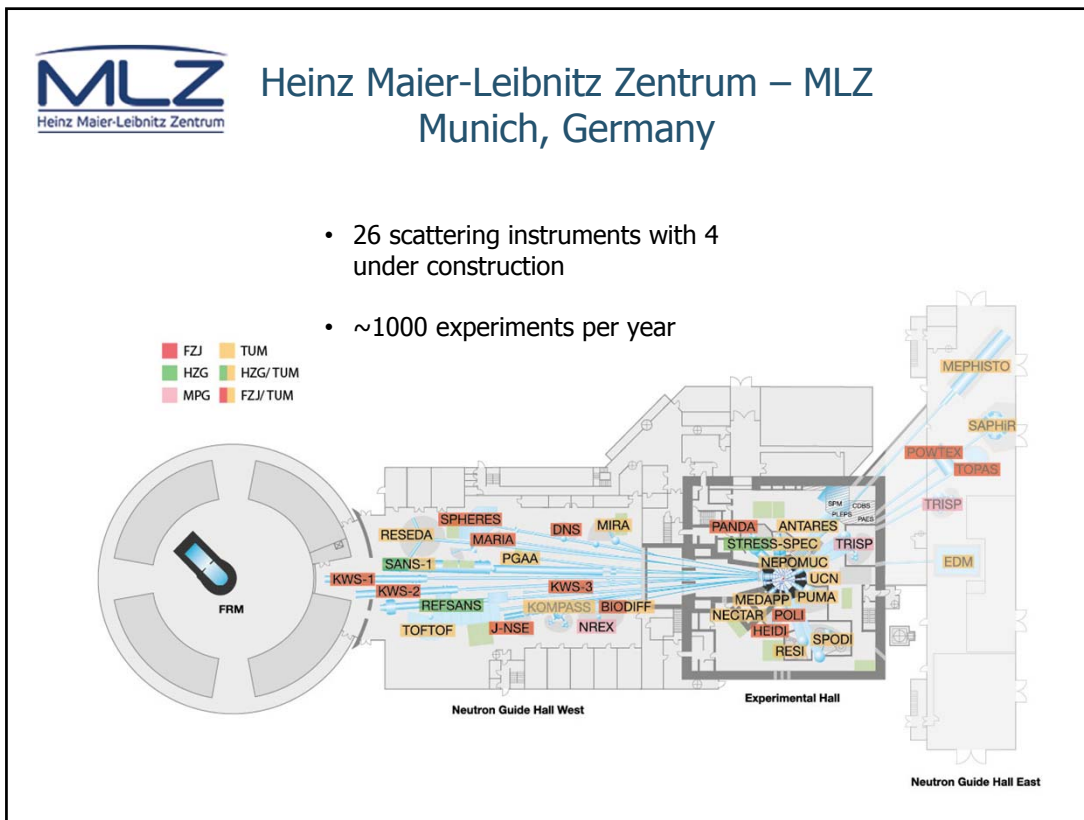


Technische Universität München

- Neutron research center based around FRM II reactor
- 20 MW open pool reactor
- Opened in 2004
- Cooperation between FZ-Julich, HZ-Geestacht and TU-Munich



- <http://www.mlz-garching.de>



## SINQ at Paul Scherrer Institut Villigen, Switzerland

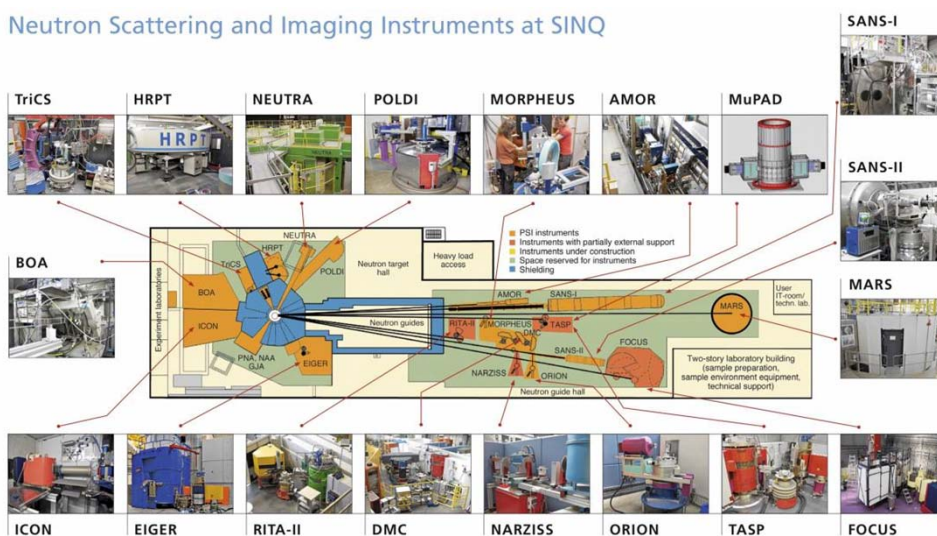


- Continuous spallation source
- 570 MeV proton beam
- 750kW
- Lead target
- Heavy water moderator and liquid deuterium cold source
- 8 Thermal beam ports plus cold guides

## SINQ at Paul Scherrer Institut Villigen, Switzerland

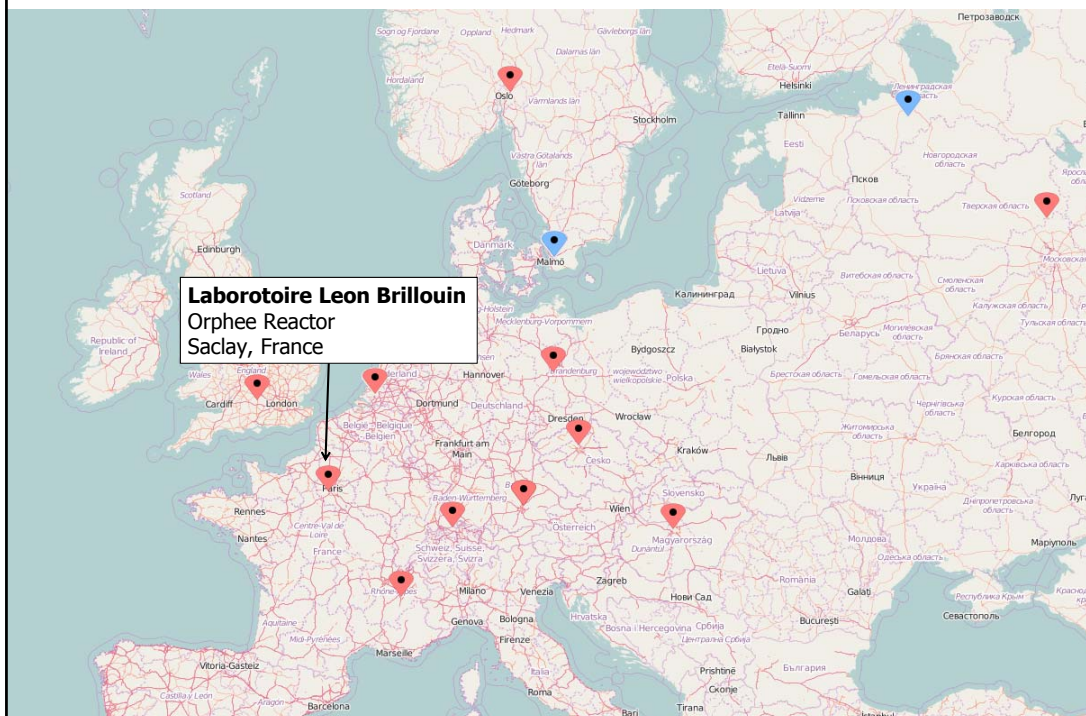
19 instruments & 4500 user visits per year

### Neutron Scattering and Imaging Instruments at SINQ

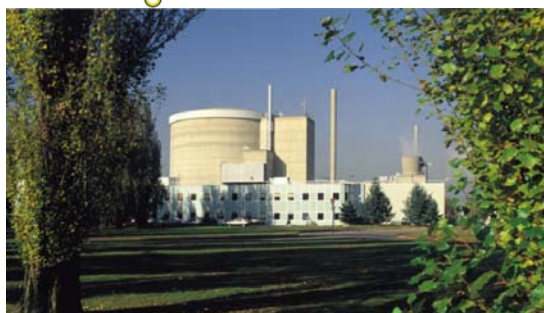


Further information: [www.psi.ch/sinq/instrumentation](http://www.psi.ch/sinq/instrumentation)

## Neutron Scattering Facilities in Europe

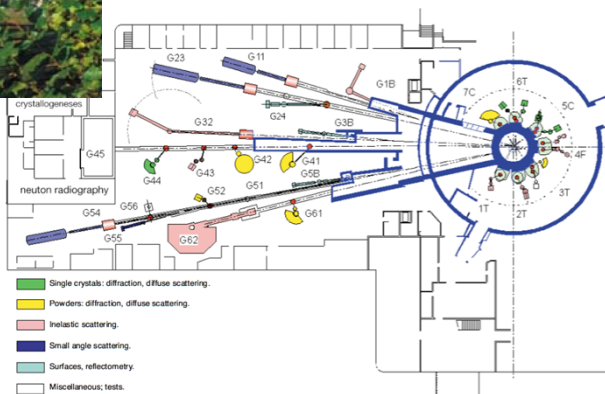


## Laboratoire Leon Brillouin Saclay, France



- 14 MW Heavy Water Reactor
- Cold source and 7 thermal beam ports
- Opened in 1980

- 25 Instruments
- ~500 users per year





## Neutron Scattering Facilities in Europe

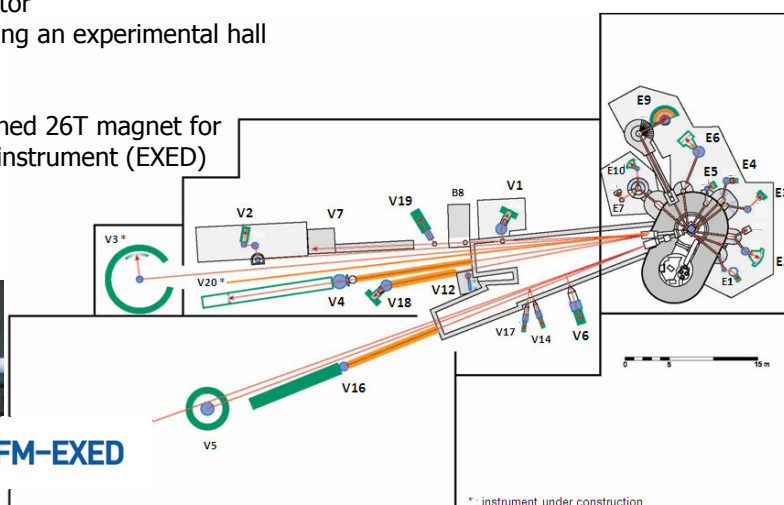


### BERII at Helmholtz Zentrum Berlin – HZB Berlin, Germany

- Opened in 1972 and renovated 1991
- 10 MW open, light water moderated swimming pool reactor
- 18 beam ports feeding an experimental hall and two guide halls
- Recently commissioned 26T magnet for extreme conditions instrument (EXED)
- 21 instruments

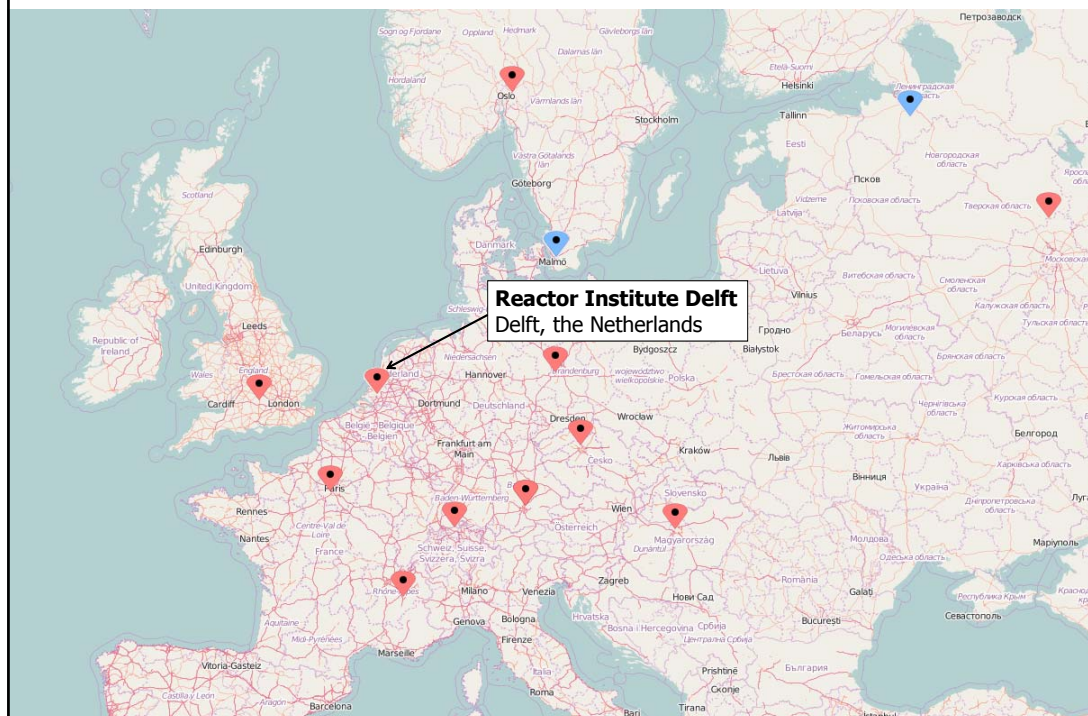


 **HFM-EXED**

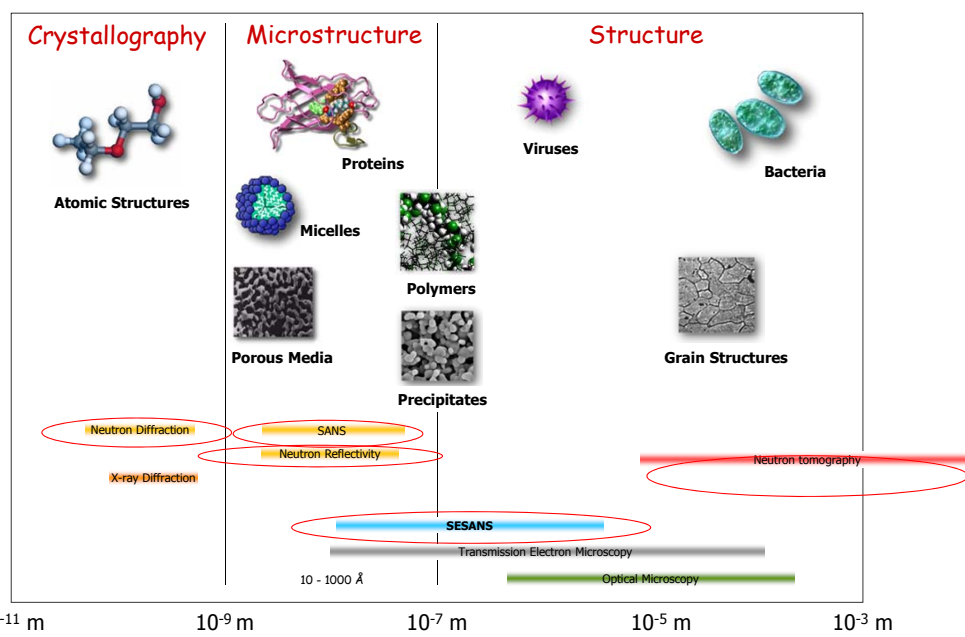


<http://www.helmholtz-berlin.de>

## Neutron Scattering Facilities in Europe

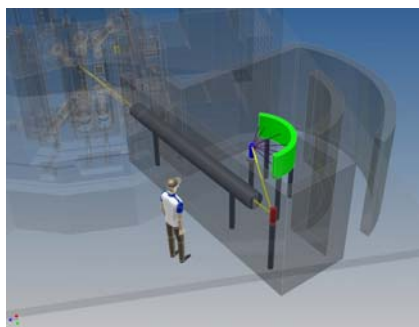
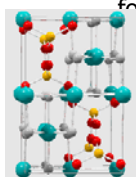


## Neutron instruments RID, Delft

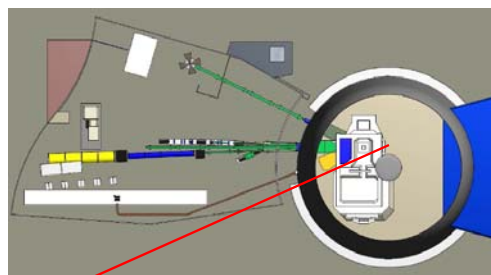


## Neutron instruments RID, Delft

**Pearl:** powder diffractometer  
for determining atomic structures

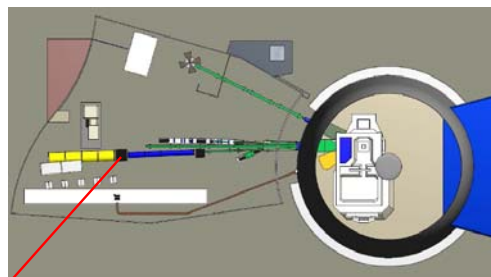


Operational since 2015



## Neutron instruments RID, Delft

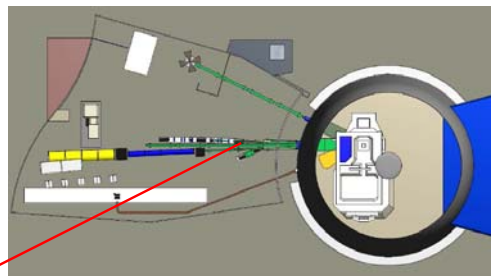
**SANS:** small-angle neutron scattering  
for determining structures on length scale 1 – 100 mm



under development

## Neutron instruments RID, Delft

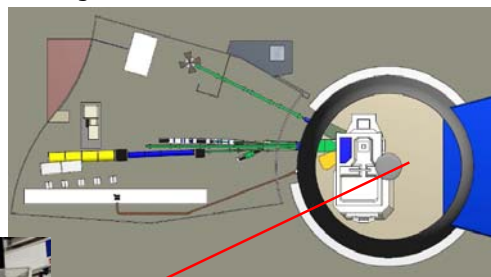
**SESANS:** spin-echo small-angle neutron scattering  
for determining structures on length scale 30 nm – 20  $\mu\text{m}$



Operational since 2002

## Neutron instruments RID, Delft

**ROG:** neutron reflectometer  
for determining thin films and interfaces length scale 1 nm – 300 nm



Operational since 1994

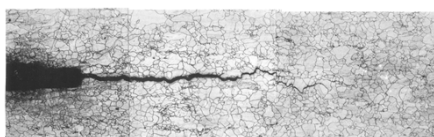


## Research Examples

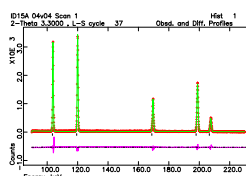
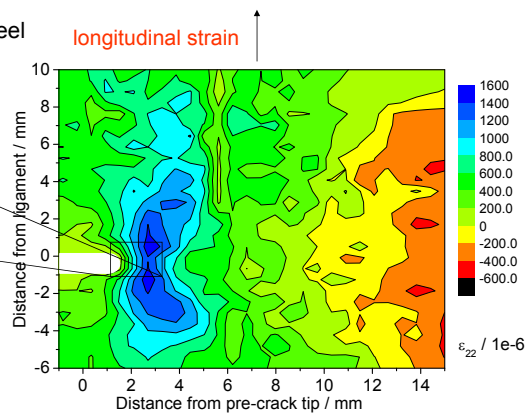
### Stress in materials

Understanding macroscopic behaviour from nanostructure

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



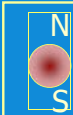
**Aim:** Exploring the boundaries of spatial resolution achievable in real materials engineering components, using combinations of in-situ techniques: imaging & diffraction, in-situ loading, high-temperature...  
**Methods:** Scanning neutron diffraction and time-of-flight imaging



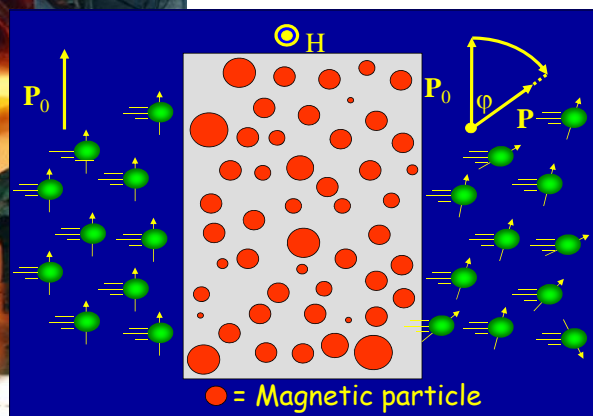
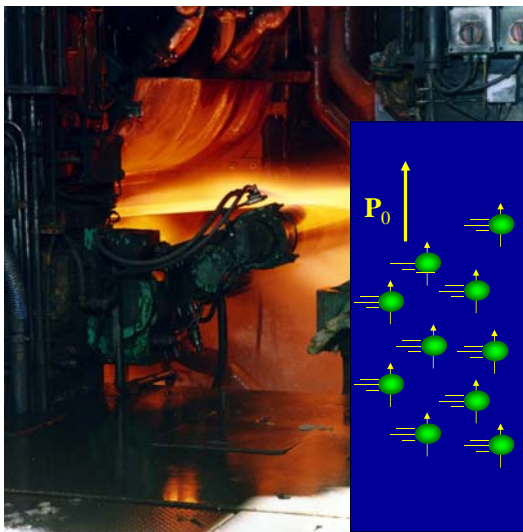
## Neutron has a spin: Larmor precession



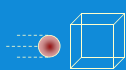
$$\frac{d}{dt} \vec{S}(t) = \gamma \vec{S}(t) \times \vec{B}(t)$$



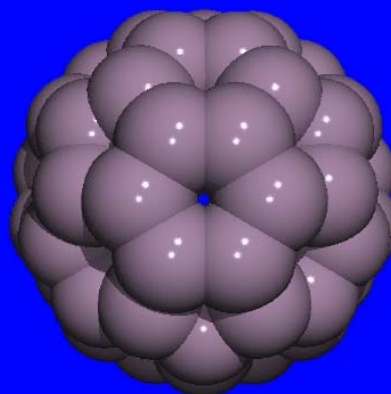
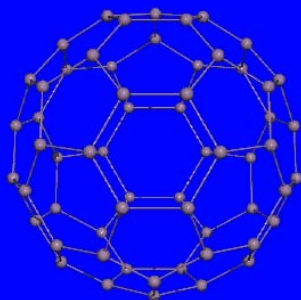
- > has a magnetic moment
- can see magnetic effects



Watching ferrite grow during austenite-ferrite transition in steels

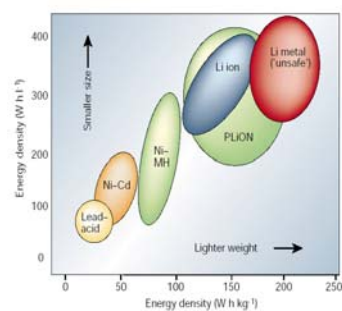
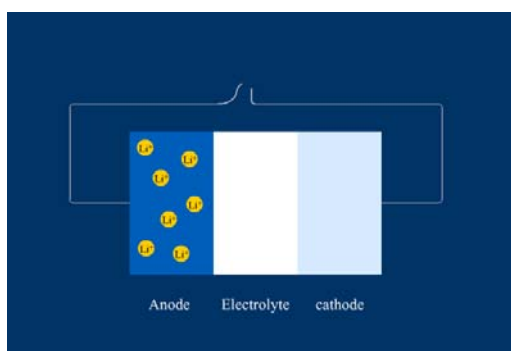


➤ Neutrons move at speeds similar to atoms – can study motion of atoms



Measuring and calculating nuclear motion – directly.

Example: Energy storage in Li-ion batteries



### Demanded properties

- High voltage difference
- High capacity
- High power density
- Long cycle life
- Low weight

### Microscopic origin

- Difference in Li-host interaction
- Amount of Li-ion stored
- Mobility of Li-ions
- Small changes in lattice parameters



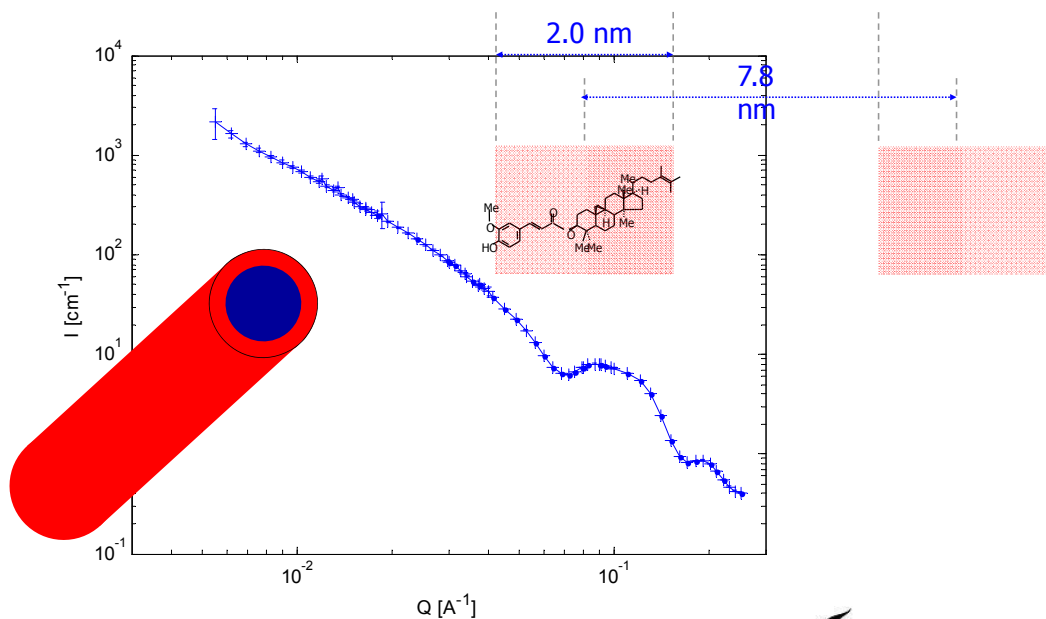
## The phytosterol compounds structure oils without solid fats



A. Bot (Unilever), *et al.*  
Faraday Discuss. **158**, 223-238 (2012)

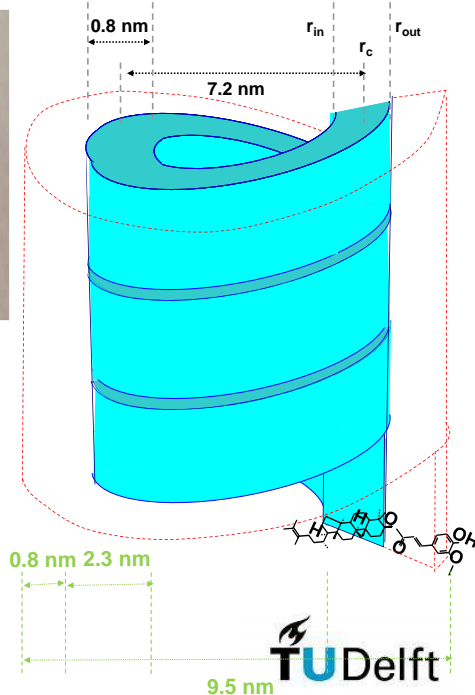
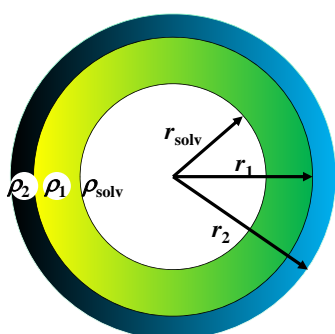
**TU**Delft

## $\beta$ -sitosterol and $\gamma$ -oryzanol in d-decane

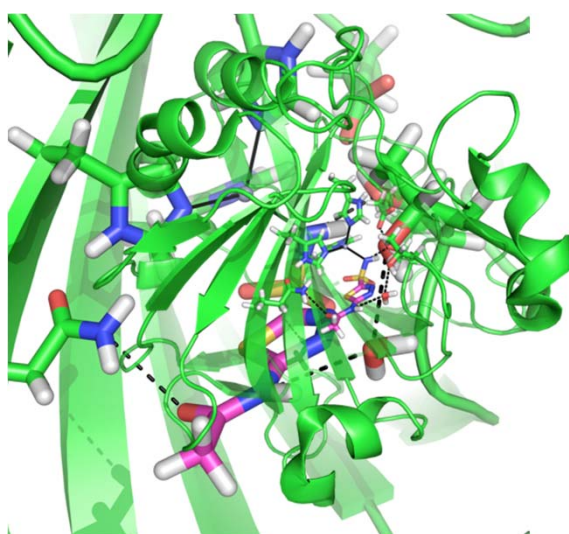


**TU**Delft

## Double walled helical ribbon



## Neutrons reveal how drugs interact with drug targets

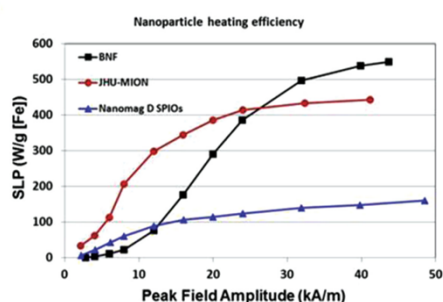


The enzyme carbonic anhydrase transports  $\text{CO}_2$  and regulates blood acidity. It is a major player in some cancers, glaucoma, obesity and high blood pressure. Neutron crystallography pinpoints protons and waters in the active site, showing how the drug Acetazolamide binds.

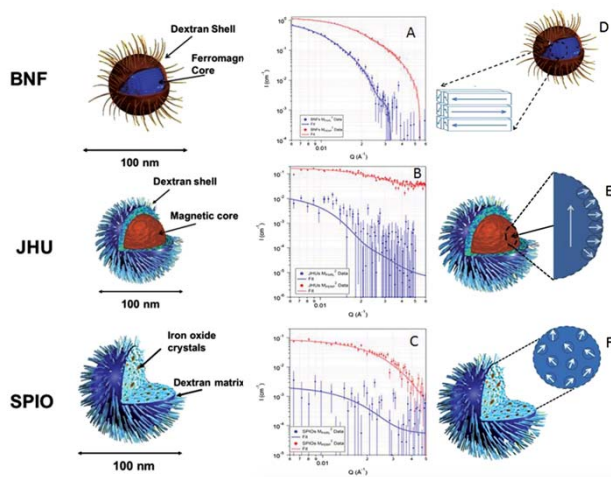
Image: Fisher, S. Z. *et al.* 2012 JACS

## Hyperthermia Treatment of Cancer

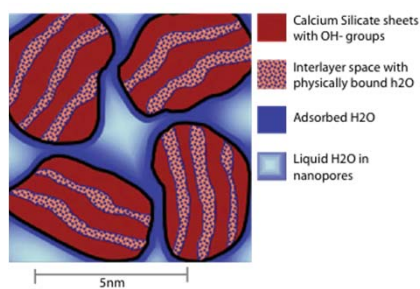
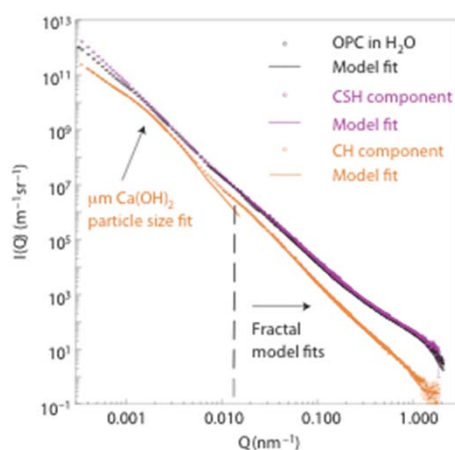
- Use magnetic nanoparticles with alternating magnetic field to locally heat tumour
- Structure of the nanoparticles has strong impact on heating response
- Use polarized neutron scattering to understand these differences



Dennis et al. *Advanced Functional Materials*, (2015), 25, 4300



## Hydration in Cement



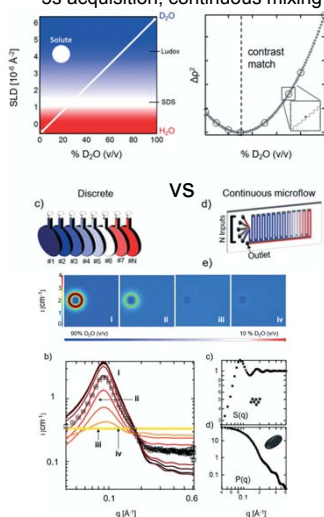
Combination of SANS/USANS and SAXS/USAXS gives detailed information about the mean formula and mass density of calcium-silicate-hydrate without drying - the first such measurement.

Allen AJ, Thomas JJ, Jennings HM. *Nature Materials*, 6(4), 311 (2007)

## Microfluidic SANS

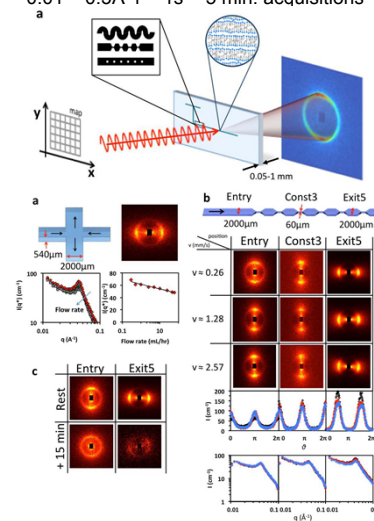
### High Throughput Mixing & Tailored Flow Geometry

400  $\mu\text{m}$  channels, 12 mm beam avg. over 20 channels  
5s acquisition, continuous mixing



Adamo, M., Poulos, A. S., Miller, R. M., Lopez, C. G., Martel, A., Porcar, L., & Cabral, J. T. (2017). *Lab Chip*, 17(9), 1559–1569.

60  $\mu\text{m}$  channels, 500  $\mu\text{m}$  beam  
0.01 – 0.3  $\text{\AA}^{-1}$  – 1 s – 5 min. acquisitions

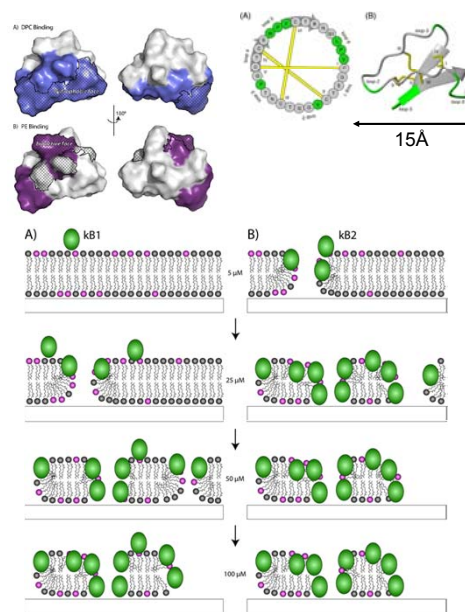
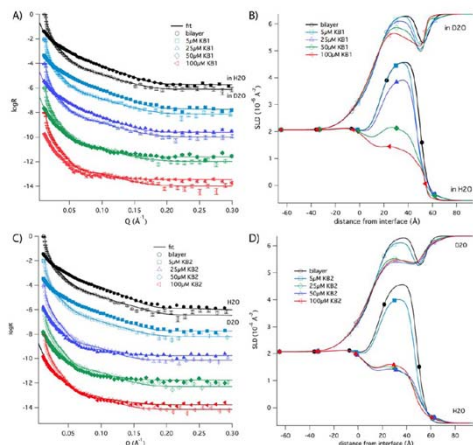


C.G. Lopez, T. Watanabe, A. Martel, L. Porcar, J.T. Cabral, *Scientific Reports*, 5 (2015) 7727.

## Kalata B1/B2 – plant cyclotides

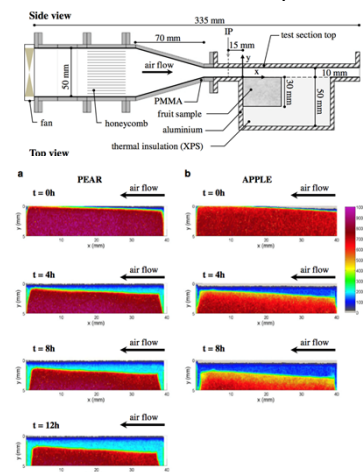
Hanna Wacklin-Knecht, ESS and Conan Wang/David Craik Institute for Molecular Bioscience, UQLD Brisbane

- Circular peptides are found in many plants – antimicrobial, anti-HIV, anticancer
- Compact structures with hydrophobic patch - oligomers in solution
- How cyclotides form pores in membranes?



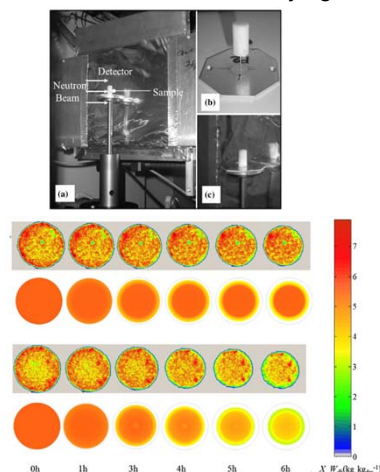
## Drying of Fruit

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



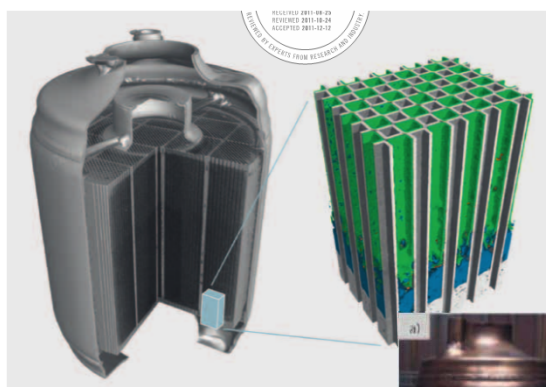
Defraeye, T., et al. *Food and Bioprocess Technology*, 6(12), 3353

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.

## Visualising Particle Distributions Using chemical sensitivity of neutrons to distinguish particle types

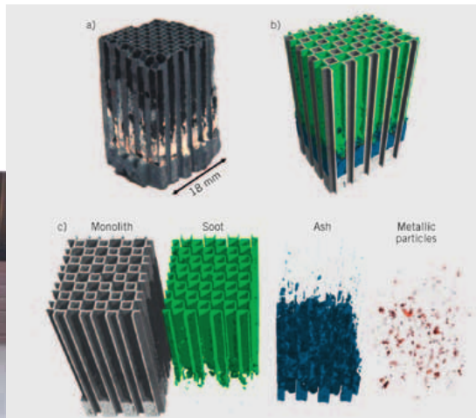


Neutron tomography used to examine particulate type and distribution in filters

**AUTHORS**  
DR. DIPL.-ING. CHRISTIAN GRÜENZWEIG

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

Neutron tomography is presently the only possibility to obtain information about



Courtesy: Ch. Gruenzweig  
PSI, Switzerland

and Applied

Fundamental Research  
with  
Neutrons

Andrew Jackson

European Spallation Source

Delivered by Wim Bouwman, Delft University of Technology

75 years of nuclear reactors: A chain reaction of applications  
KIVI-NNS Symposium, 3rd November 2017