Neutron scattering:
a tool for materials investigations

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University of Tartu

Kim Lefmann

Short presentation

- Kim Lefmann
- Danish, 53 years

- Ph.D. 1995 physics (NBI), U. Cph.
- Post doc, Helsinki U. Techn. 1995-96
- Senior Scientist at Risø 1997-2008
- Ass. Prof., NBI, Univ. Cph. 2008-

- Board of the Danish neutron/X-ray instrument center, DANSCATT
- Leader of the NNSP Neutron School

- Favorite techniques:

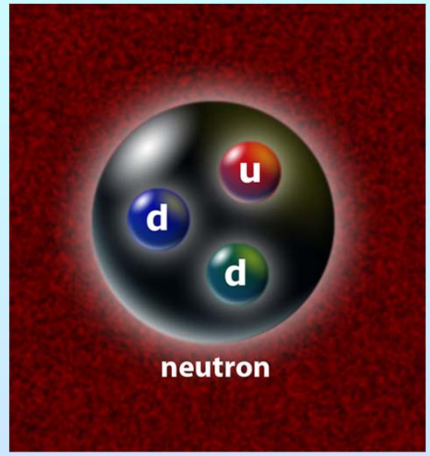
Neutron scattering
Numerical simulations
Low temperature techniques

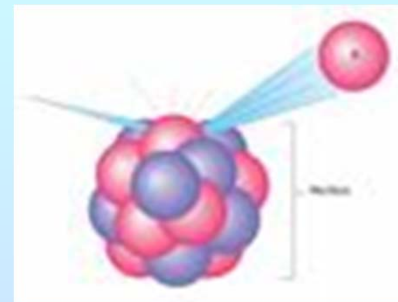
- Research interests:

Quantum magnetism
Frustrated magnetism
Multiferroics
Nanoscale magnetism
Superconductivity
Instrumentation

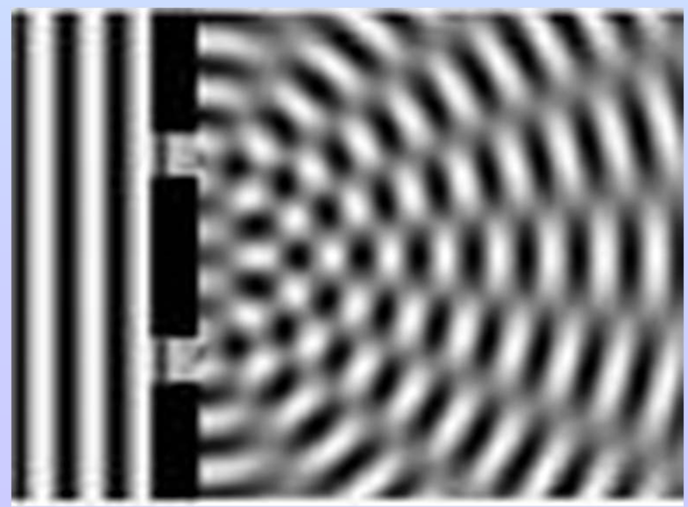
What is a neutron?

- A part of the atomic nucleus
  - Made of 3 quarks
  - Mass and spin like the proton
  - Electrically neutral
- Can react with nuclei
- Can scatter off nuclei





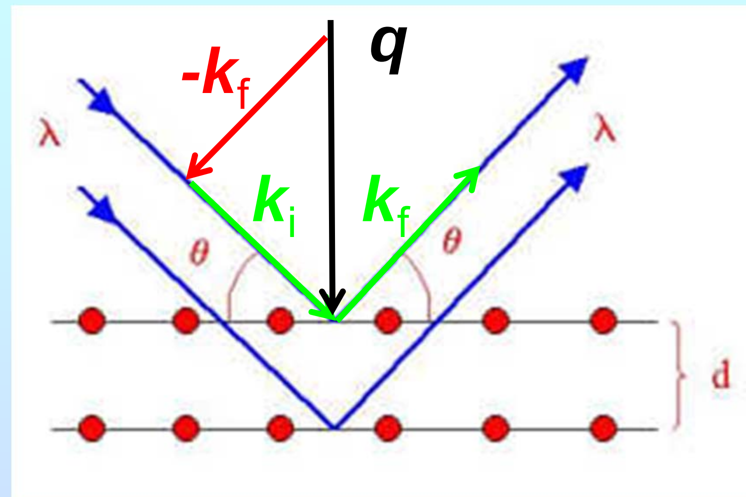
- A slow neutron behaves as a wave
- Interference !
- Used to investigate
  - Chemical composition
  - <u>Materials structure and properties</u>



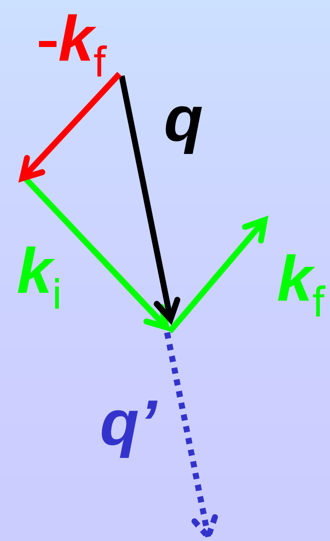
Elastic and inelastic scattering

- **Elastic:** Bragg law $n\,\lambda = 2\,d \sin\theta$
- Wave number $k = 2\,\pi\,/\,\lambda$
- Scattering vector $\boldsymbol{q} = \boldsymbol{k}_i - \boldsymbol{k}_f$

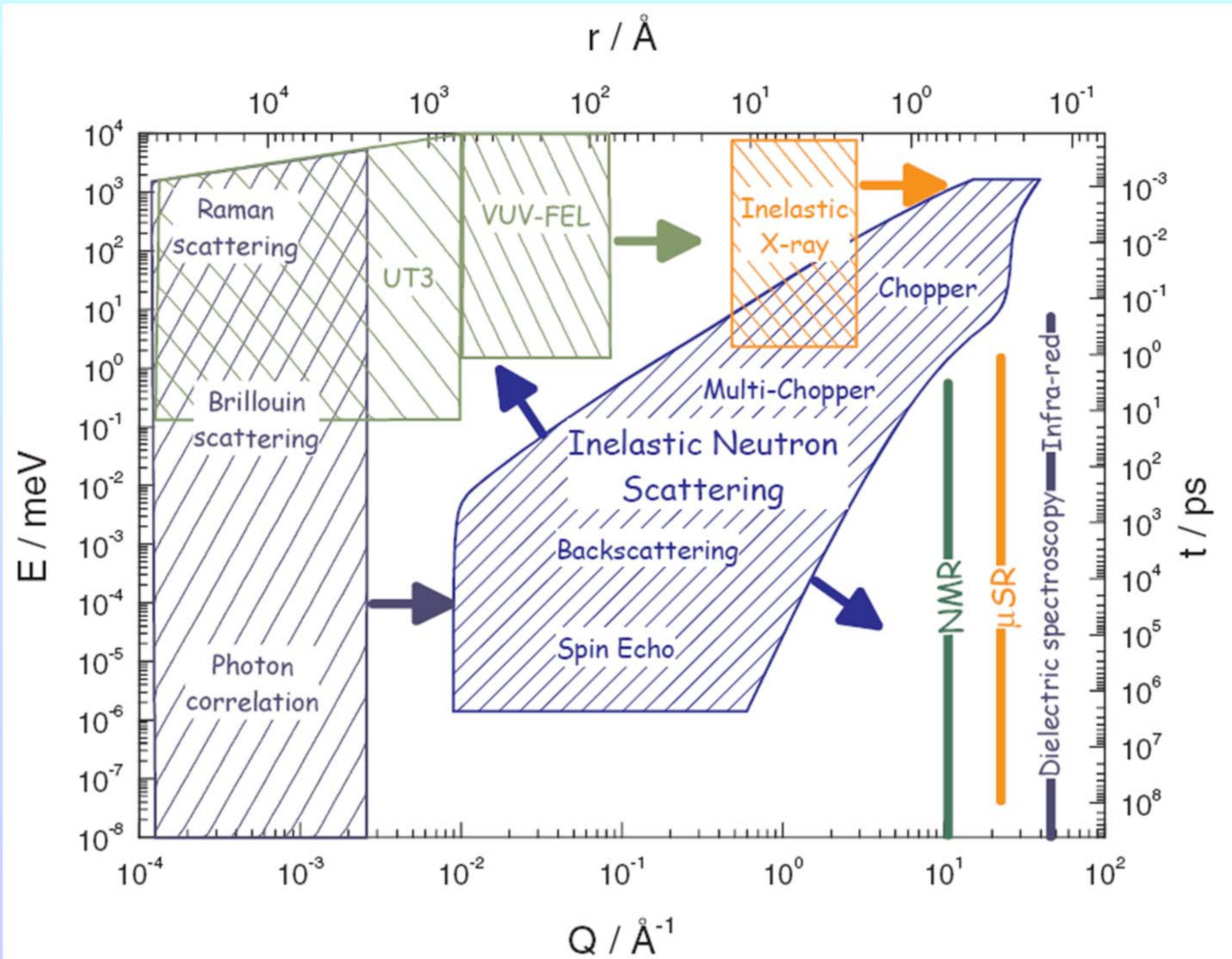
$$= 2\,\pi\,/\,d$$



- **Inelastic:** Conservation laws
- Energy transfer: $\hbar\omega = E_i - E_f$
- Energy conservation $\hbar\omega = \hbar\omega(\boldsymbol{q}')$
- Momentum conservation $\boldsymbol{q} = \boldsymbol{q}'$



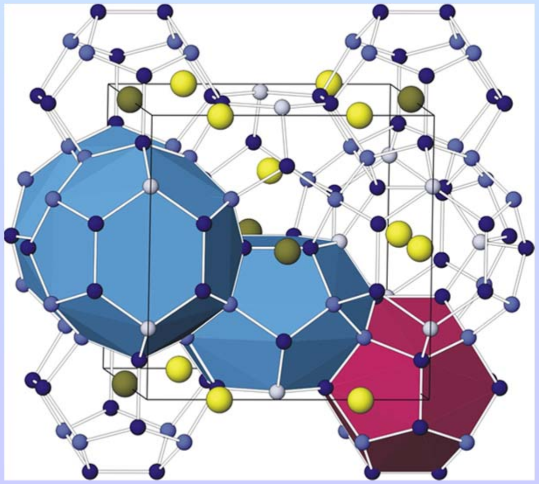
E- and q-coverage



Why neutrons ? (1)

The neutron has a wavelength (Å) and an energy (meV) comparable to typical atomic spacings and vibrational energies -

so you can study both atomic structure and dynamics (simultaneously if required)



Neutrons tell you 'where the atoms are and what the atoms do'
(Nobel Prize citation for Brockhouse and Shull 1994)

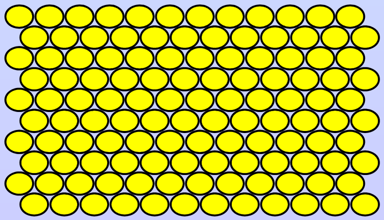
M. Christensen (AU Chemistry), Nature Materials 2008

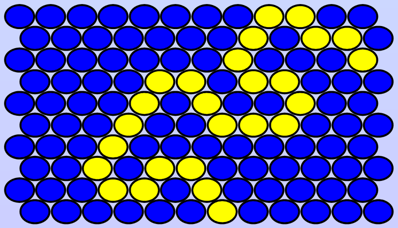
Why neutrons ? (2)

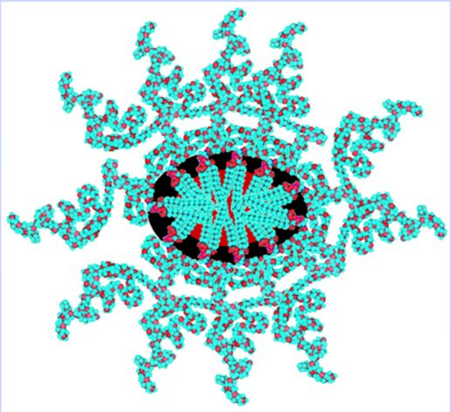
The neutron scattering cross-section varies randomly through the periodic table and is isotope dependent -

distinguish light and heavy atoms
or atoms of similar Z

enabling the technique of
isotopic substitution/contrast variation





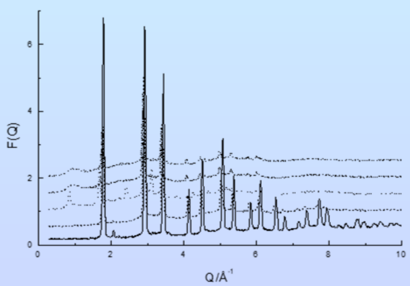


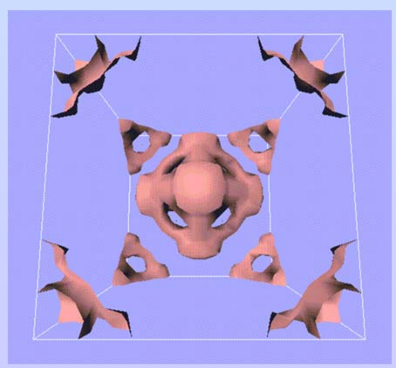
L. Arleth, KU NBI

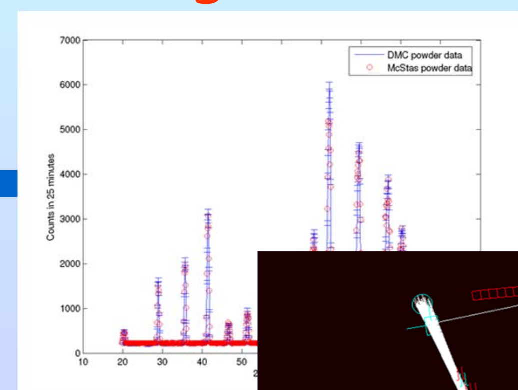
Why neutrons ? (3)

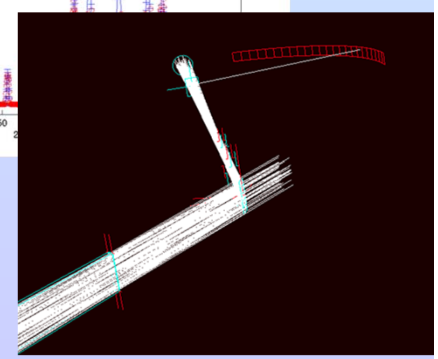
The neutron is a weak probe -

giving a direct and quantitative link with theory and computer simulation/modelling







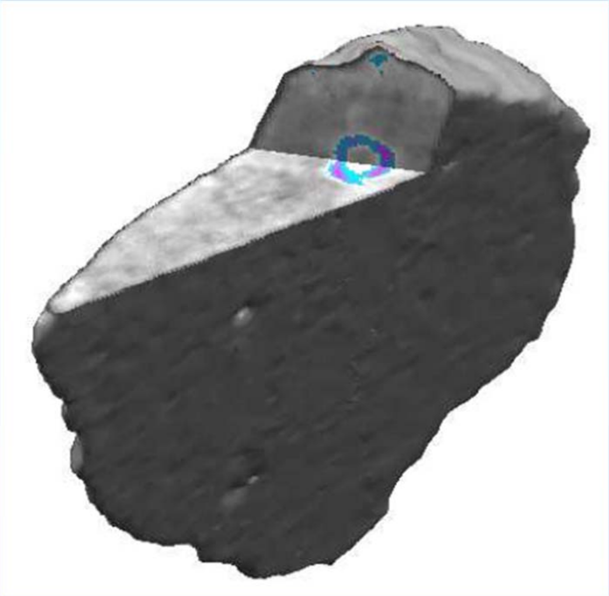


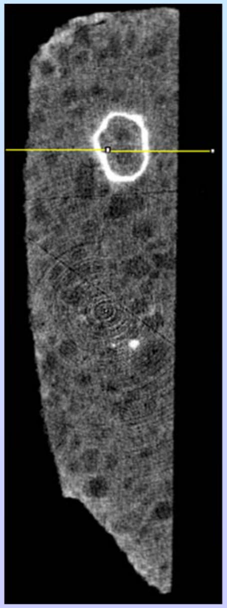
P.K. Willendrup, E.B. Knudsen,
K. Lefmann et al
McStas, DTU-KU software

Why neutrons ? (4)

The neutron is highly penetrating -

enabling studies of thick samples
and samples in complex sample environment





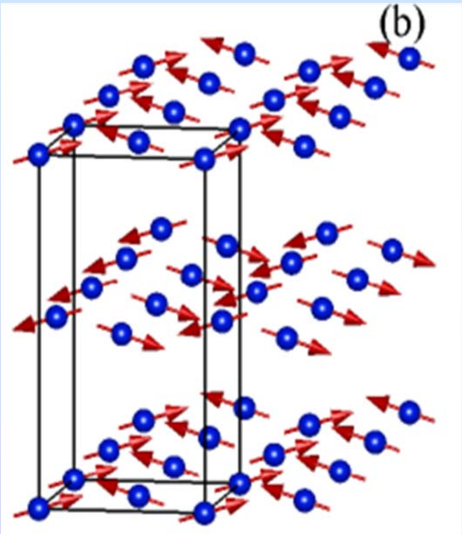
H. Haack et al,
science museum 2005

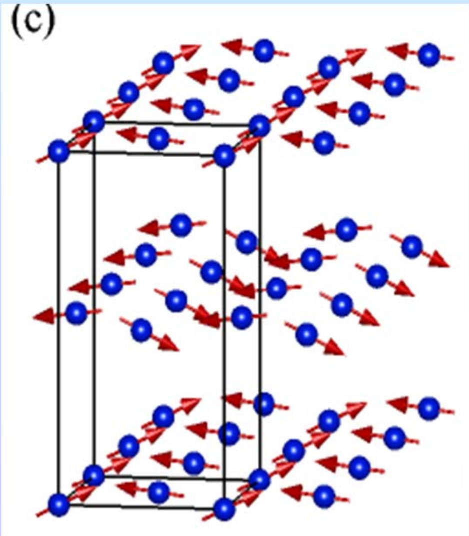
15 T magnet, PSI, 2004
(Carlsberg and FNU)

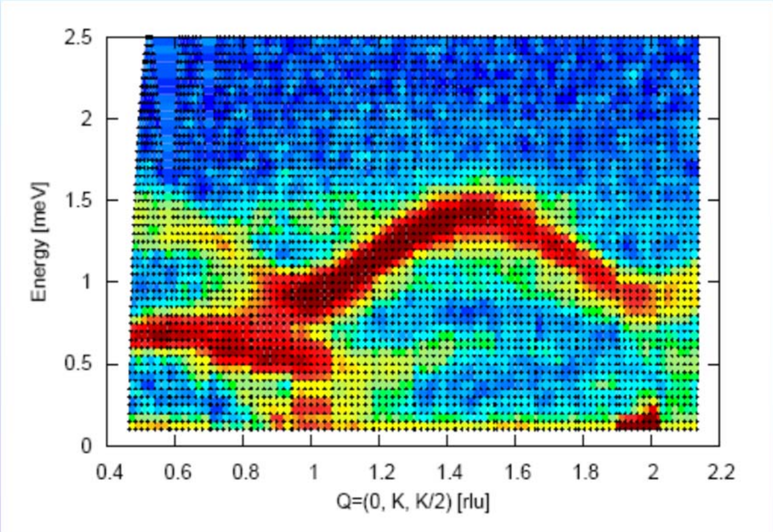
Why neutrons ? (5)

The neutron has a magnetic moment but no charge -

enabling studies of magnetic structure and dynamics



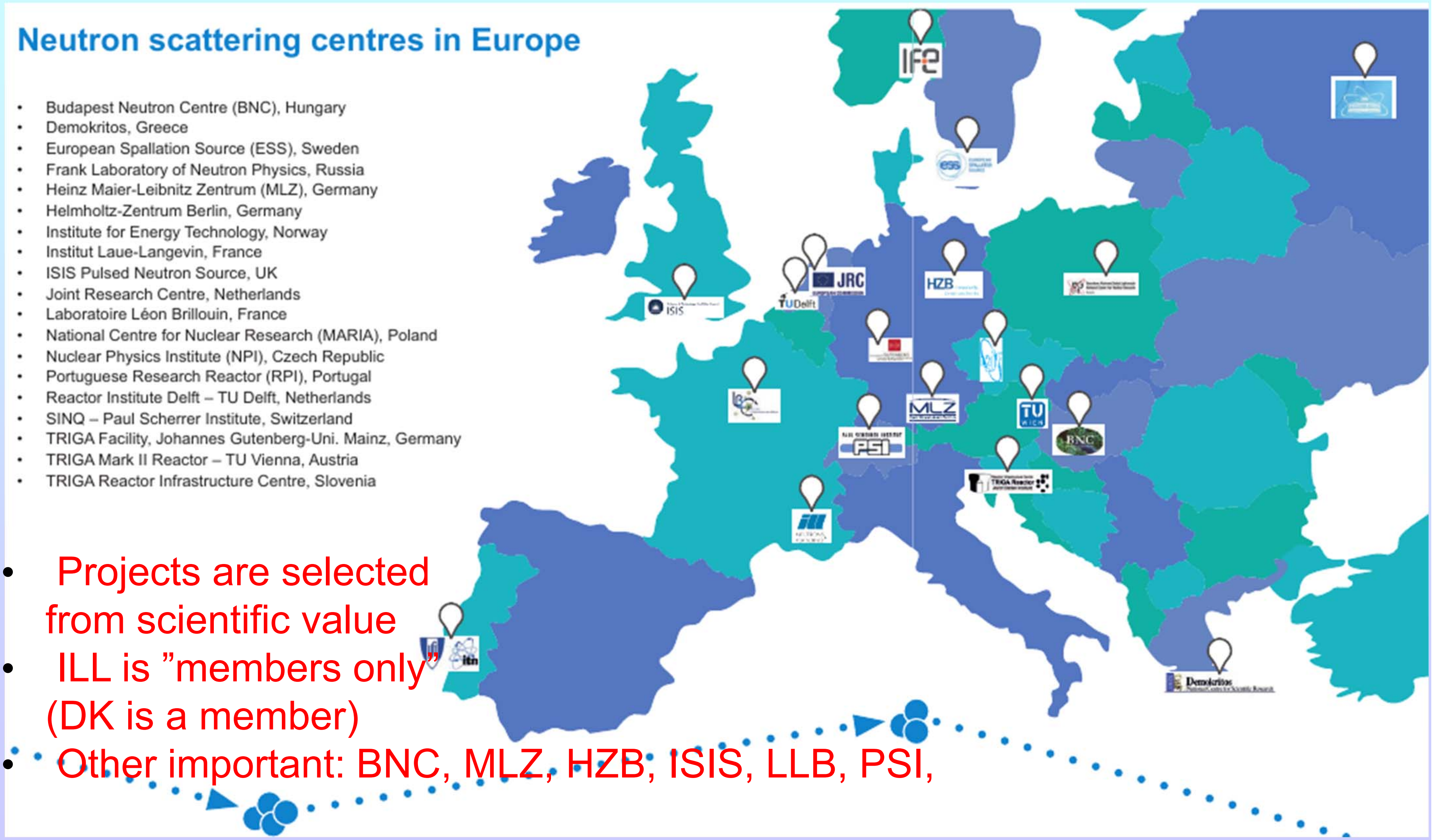




T. B. S. Jensen et al, Risø, Phys Rev B 2008

Student team, KU, NBI, 2005
-> C. Bahl et al, Physica B, 2007

European neutron facilities



- Projects are selected from scientific value
- ILL is "members only" (DK is a member)
- Other important: BNC, MLZ, HZB, ISIS, LLB, PSI,

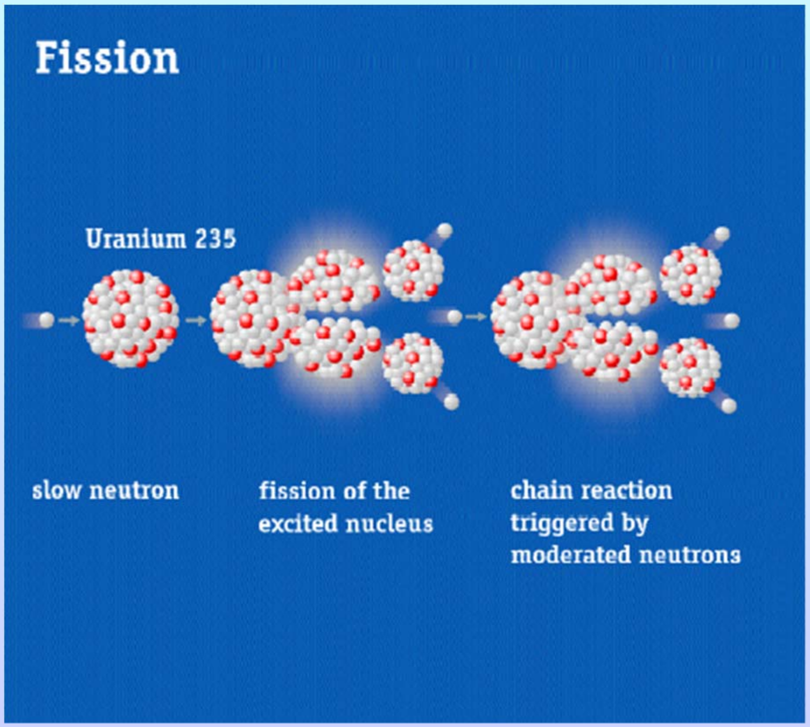
ILL – the neutron Mekka

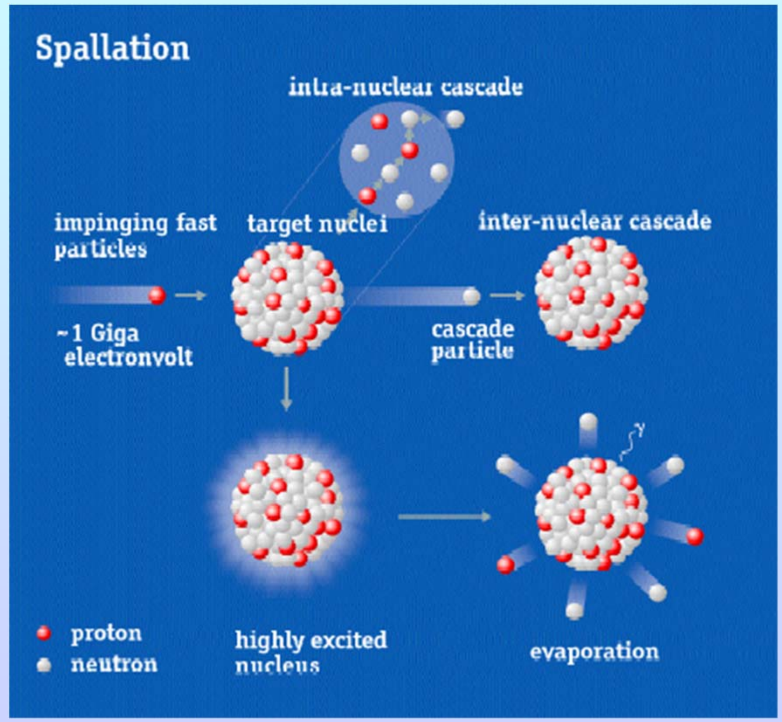
Owned by: UK, D, F
Members: 12 other countries

DK and S are members

2015 (typical year):
- 40 instruments
- 834 experiments
- 4184 instrument days
- 1386 users
- 556 publications

Production of neutrons

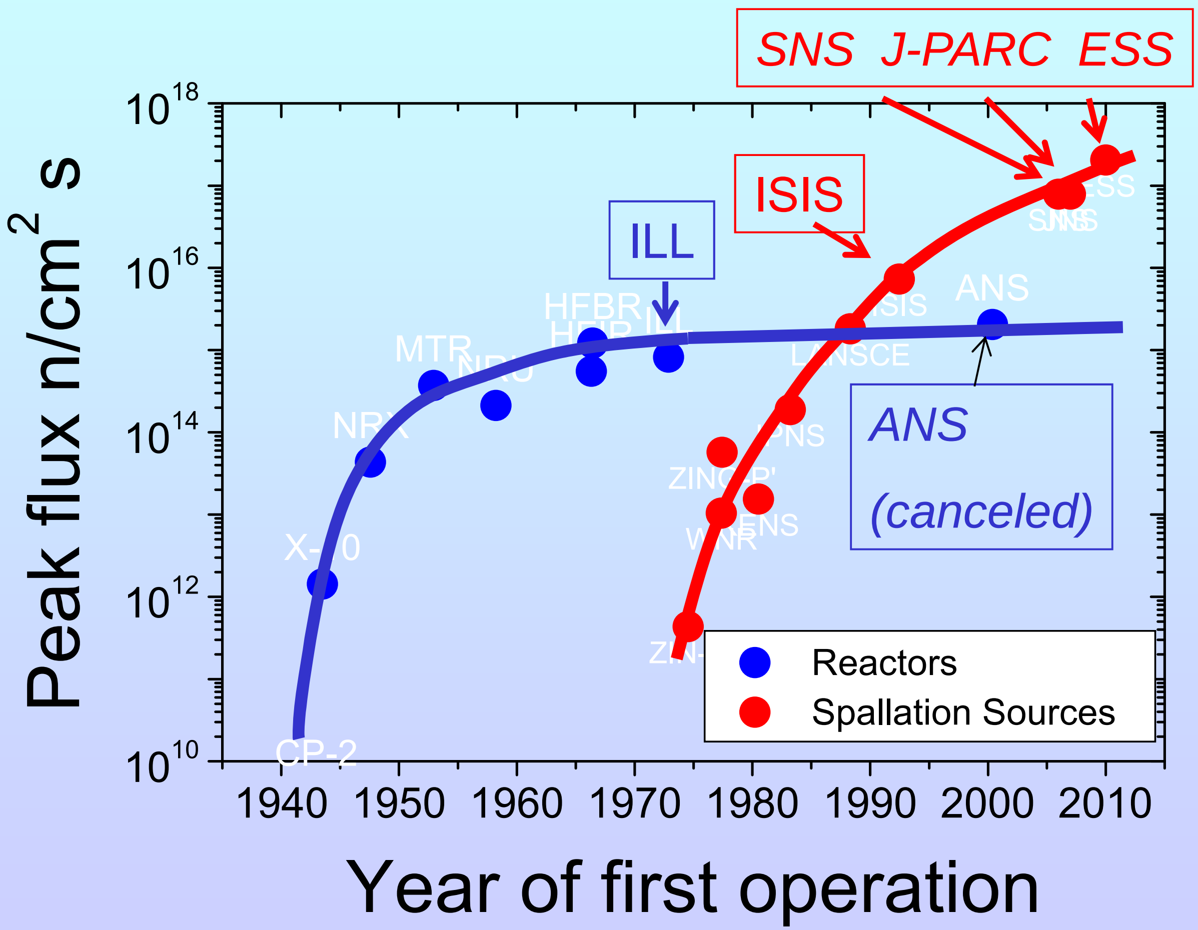




Traditional, nuclear reactor

Modern, proton accelerator

Intensity vs time



- Neutron scattering suffers from lack of intensity
- What does the future bring?

SNS, Oak Ridge, Tennessee

- Short-pulses
- 1.4 MW
- 20 instruments
- First neutrons April 2006
- Users from 2008

- World leading

- ... together with Japanese project J-PARC

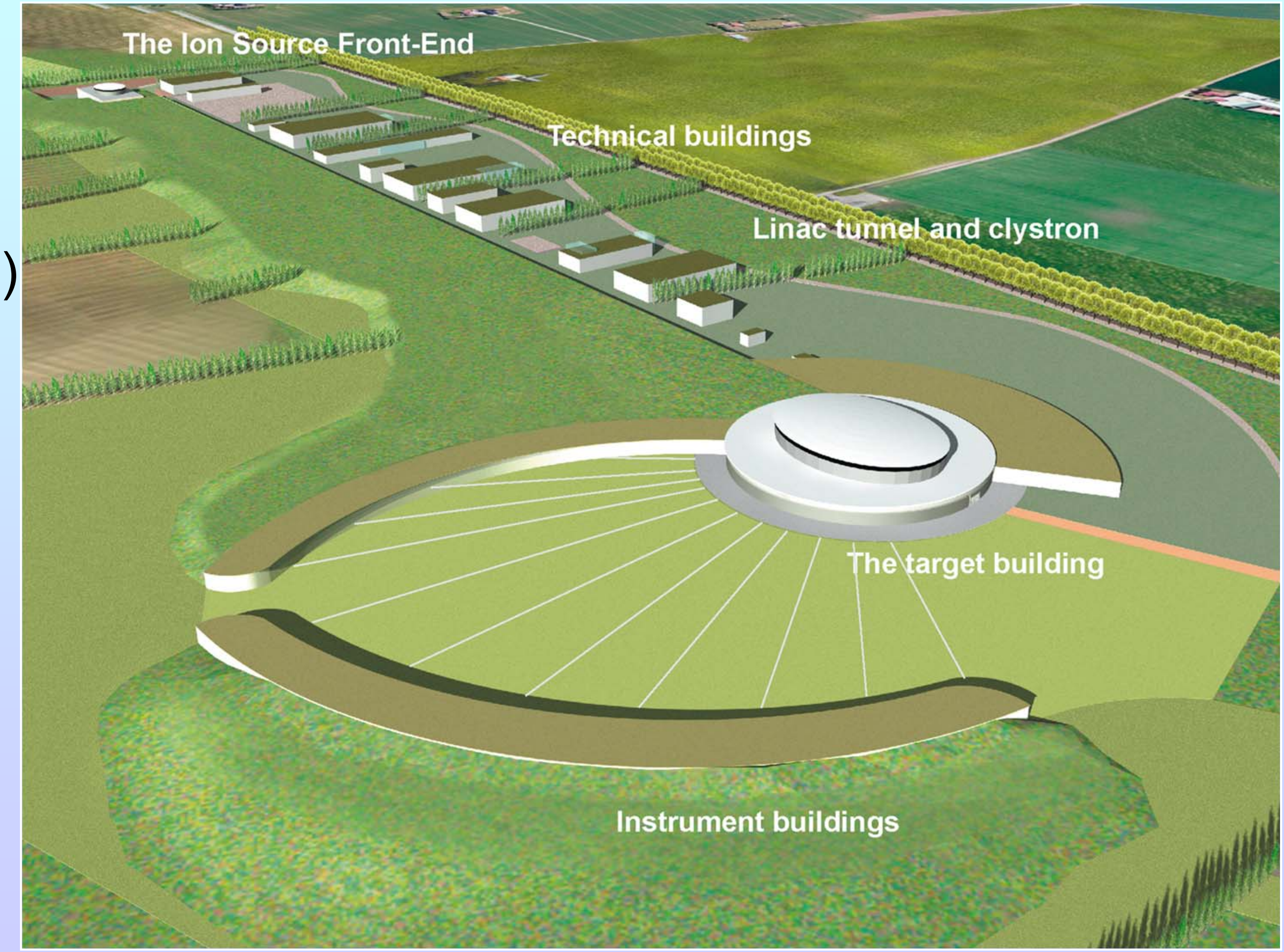
The ESS project

Accelerator:
• Length: 600 m
• Protons: 2.0 GeV
• Power: 5 MW

Neutrons:
• Long pulses (2.86 ms)
• 15 (22+) instruments
2 DK-N instruments
• 10 × SNS

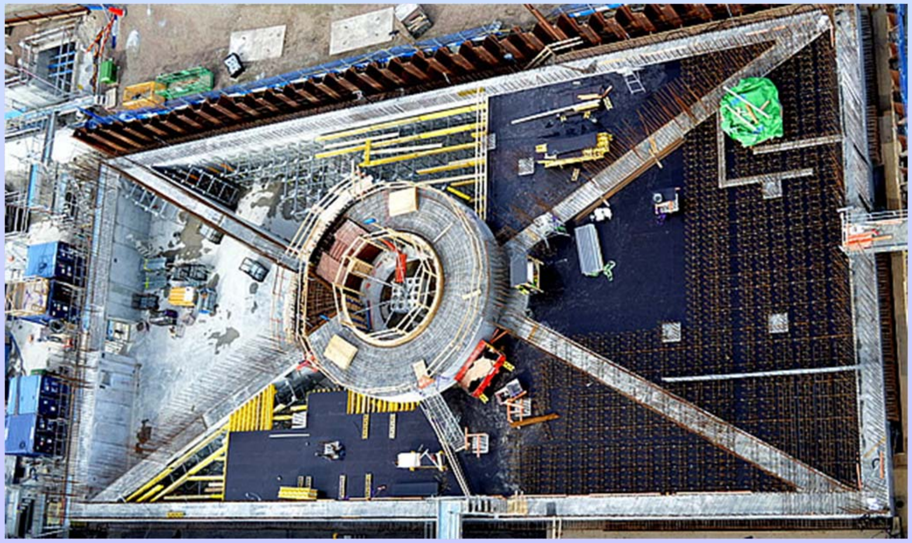
Construction:
• 2014-2020 (2025)
• 1.843 G€

Site contenders:
• Bilbao (E)
• Debrechen (H)
• Lund (S)



28/5-2009 Bruxelles: Lund chosen as ESS site
4/7-2014: Final building decision !

Recent ESS photos



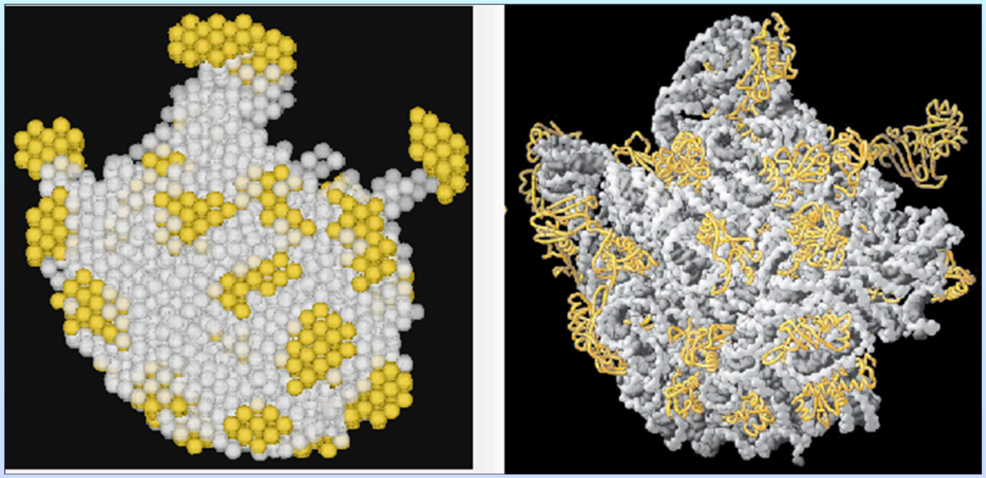
Neutrons for many fields of science

- Condensed matter physics
  (magnetism, superconductivity, glasses, liquids)
- Materials research
  (stress/strain, hydrogen in materials)
- Soft condensed matter
  (polymers, composites)
- Structural chemistry
  (catalysis, reactions, parametric studies, molecular spectroscopy)
- Geology
  (minerals at high P,T, hydrogen in rocks)
- Life sciences
  (membranes, protein structure, -dynamics, and -complexes)
- Nanoscience (most of that above)
- Particle physics
  (basic properties of the neutron, basic quantum mechanics)

Protein Crystallography by small angle neutron scattering

Determination of Protein confor-mations in solution

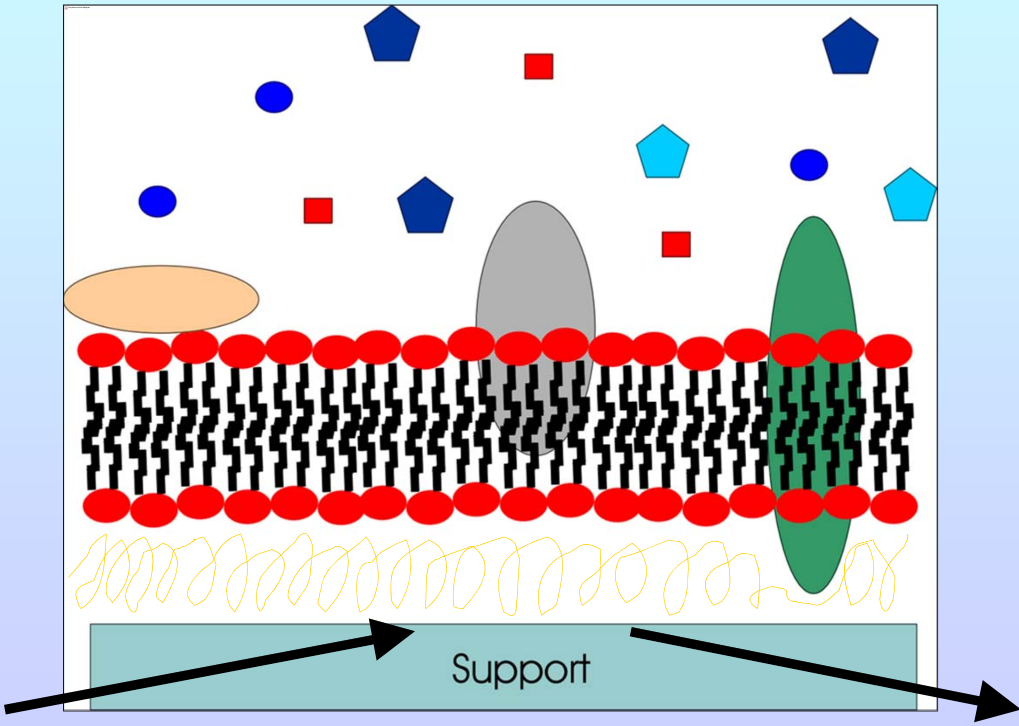
H-D substitution:
- Partial labeling of functional groups
- Improved contrast situation



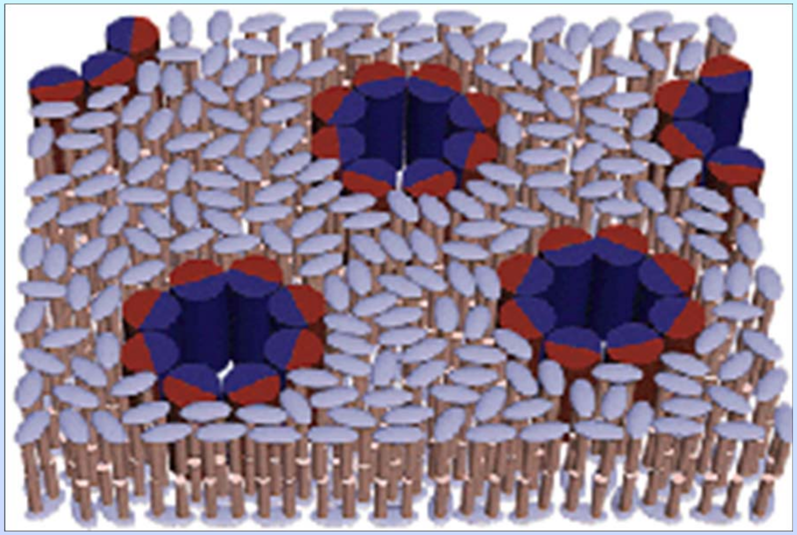
The 50S subunit in the map of the 70S E.coli ribosome.
Left: Neutron data; solution scattering
Right: X-ray crystallography

Biological Membranes

Native Membranes and Biosensors



Neutron reflection



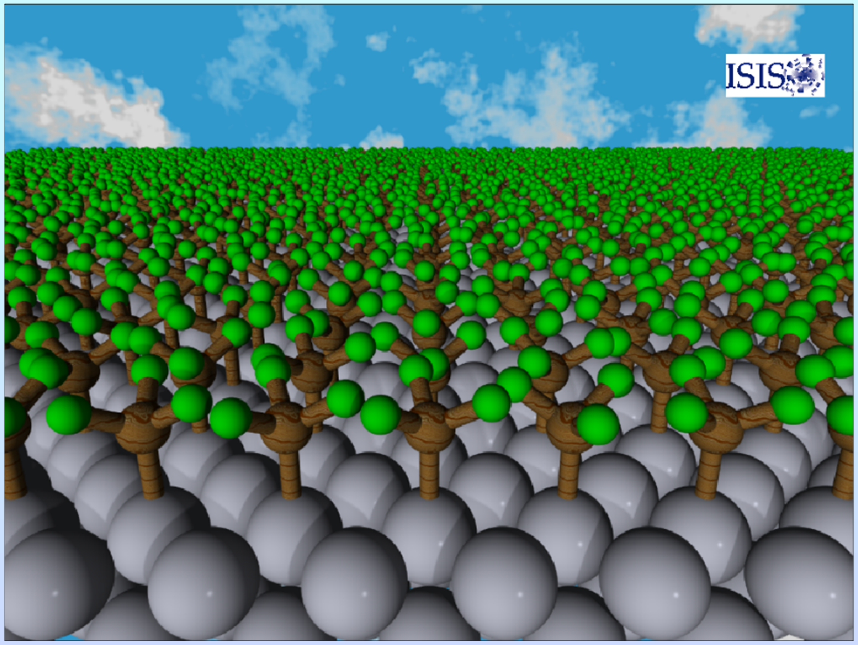
structural investigations
in active state

Studies of catalysis

Penetration: In-situ studies of catalytic processes

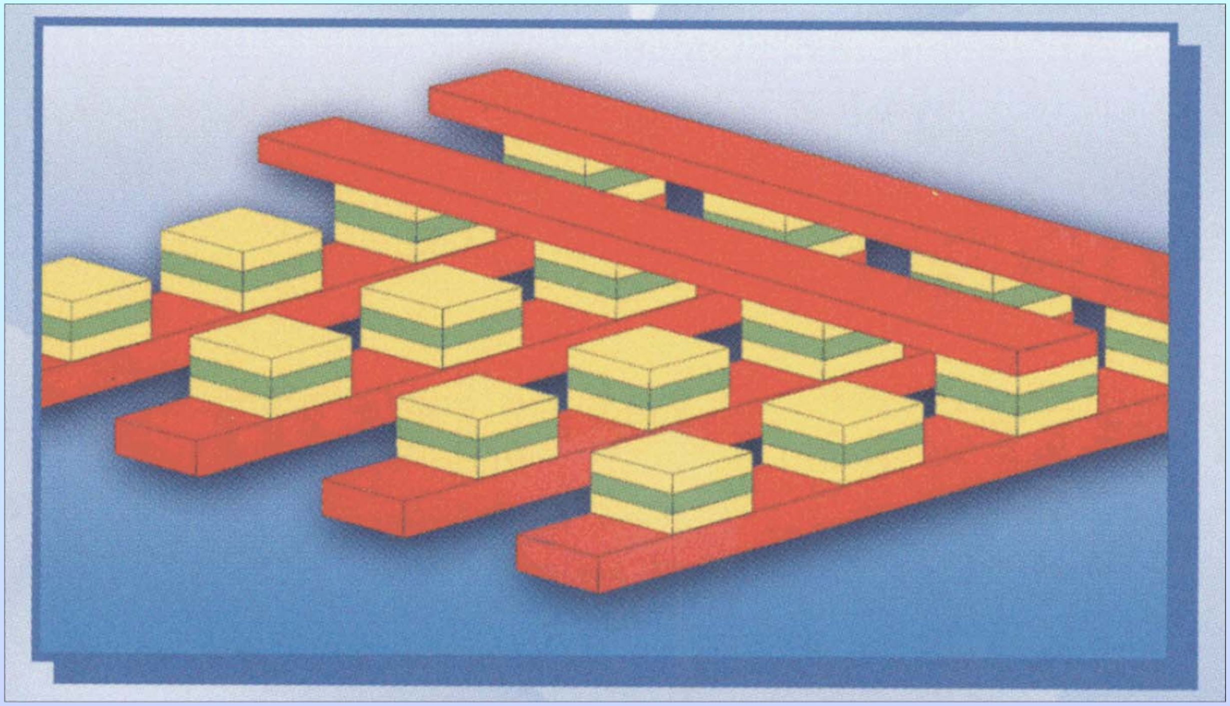
Flux: Real sized reactors can be studied

Instruments: Spectroscopy of reaction intermediates, with or without H



Artists view of a Palladium catalyst, passivated by methyl groups. Studied by molecular spectroscopy at ISIS

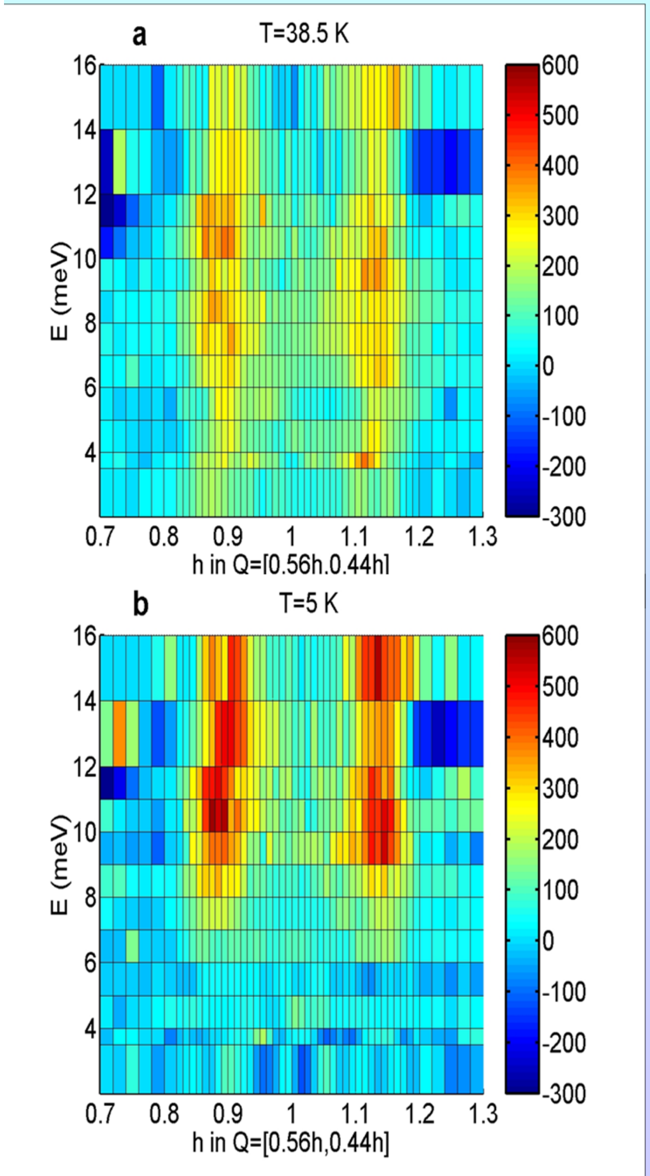
Magnetoelectronics



Nanosized magnetic storage devices.

Investigation of spin-reversal and spin-dynamics in magnetic nanostructures by inelastic neutron scattering

Magnetic fluctuations in superconductors



- Simple cuprate HTSC $(La_{2-x}Sr_x)CuO_4$
- Superconducting below 38 K - why?
- has incommensurate magnetism (antiferromagnet with long repetition)
- These data: x = 0.16 (optimal doping)
- Short range fluctuations; nm range
- A gap in the fluctuation spectrum opens up in the SC phase
- Magnetism connected with HTSC!

B. Lake et al, Nature (1999); Science (2001); Nature (2002)

B. Lake et al, Nature Materials (2005)

N.B. Christensen et al, Phys. Rev. Lett. (2004)
J. Chang et al, Phys. Rev. Lett (2009)
A. Tranum-Rømer et al, Phys. Rev. B (2013)
L. Udby et al, Phys. Rev. Lett. (2013)
... many theory papers by B.M. Andersen and P. Hedegård