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Accelerator-based neutron sources for condensed matter research - Cockcroft Institute Lectures 2015

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Accelerator-based Neutron Sources for Condensed Matter Research – Cockcroft Institute Lectures 2015

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These lectures provide a self-contained introduction to the use of accelerator-based neutron sources for condensed matter research. In their present form, they were first given in 2015 as part of the *Applications of Accelerators* graduate course at the *Cockcroft Institute of Accelerator Science & Technology*, Daresbury Laboratory, United Kingdom. They also build on previous teaching materials prepared for the graduate curriculum of the *The John Adams Institute for Accelerator Science* at the University of Oxford. The first lecture is primarily concerned with neutron production. It sets the scene by reviewing the merits and strengths of neutron-scattering as a condensed-matter probe. It then explains the reasons behind the increasing use of accelerator technology to this and other ends, including muon production. A number of recent and ongoing projects around the globe to develop both small- and large-scale accelerator-driven neutron facilities are described, alongside emerging concepts aimed at the optimisation of neutron production for specific scientific applications. The second lecture provides an overview of condensed matter research with neutrons across a number of disciplines in science and engineering. Key concepts are illustrated using recent case studies primarily carried out at the *ISIS Pulsed Neutron & Muon Source*, Rutherford Appleton Laboratory, United Kingdom. We close by presenting a number of opportunities on the horizon, in order to address emerging research trends in condensed matter and stimulate further work in the field of accelerator science.

These lectures provide a self-contained introduction to the use of accelerator-based neutron sources for condensed matter research. In their present form, they were first given in 2015 as part of the *Applications of Accelerators* graduate course at the *Cockcroft Institute of Accelerator Science & Technology*, Daresbury Laboratory, United Kingdom.[1] Course materials have been primarily drawn from: the recent thematic volume *Neutron Scattering – Fundamentals*;[3] a number of lectures and courses given at the *The John Adams Institute for Accelerator Science* at the *University of Oxford*,[2] *University College London*,[4] *Università degli Study di Milano – Bicocca*,[5] and *Università di Roma – Tor Vergata*;[6] as well as recent research carried out primarily at the *ISIS Facility*[7] and the *ISIS Molecular Spectroscopy Group*.[8–12] The primary target audience in mind is the graduate or advanced undergraduate student in accelerator science who wishes to gain familiarity with the use of charged-particle beams for neutron production and the rationale behind such a choice. Each lecture has been designed to last for approximately one hour and assumes a basic (undergraduate) level of understanding of condensed-matter physics and chemistry.

Lecture I (Neutron Production) sets the scene by providing a brief introduction to the use of neutrons for condensed-matter research, as the technique *par excellence* to investigate *where atoms are* (structure) and *what atoms do* (dynamics), a popular motto across generations of neutron-scattering practitioners. The complementarity with other techniques is also highlighted, particularly in the study of light elements like hydrogen or magnetic phenomena, both at the heart of topical research areas such as energy conversion and storage (e.g., battery materials) and data storage (e.g., hard-drives). Neutron production is then presented in a chronological fashion, from the pioneering work that led to the discovery of this elusive particle in the 1930s,[13,14] to the advent of intense neutron sources over the past seventy years. We discuss the primary differences between fission-based research reactors and accelerator-driven facilities, and explain how the past two decades have witnessed a golden age of the latter approach leading to an unprecedented increase in capacity using spallation techniques, as described in more detail in *Chapters 1-3* in Ref. 3. Taking the *ISIS Facility*[7] as an example of a world-leading spallation neutron source which continues to evolve after three decades of uninterrupted operation, we describe in some detail how it works, from ion production and acceleration all the way to neutron moderation and transport to the point of use in an instrument. As interlude, we also provide a brief introduction to muon production and use, along with selected examples of muon science. This discussion is followed by a description of other major sources around the world including *SINQ* in Switzerland,[15] *SNS* in the USA,[16] *MLF* in Japan,[17] *CSNS* in China,[18] and *ESS* in Sweden.[19] We also cover parallel efforts worldwide to develop medium-size[20–23] and compact[24,25] neutron sources for specific applications, examples of which include the recently commissioned *RIKEN Accelerator Neutron Source*.[26] This discussion also brings to the fore a major distinction between neutrons and photons – in the former case, lab-based sources (as opposed to dedicated central facilities) remain to be developed, and accelerator technologies offer a number of yet-to-be-tapped opportunities for further R&D work.

Lecture II (Neutrons for Science) presents in some detail the operation of a large-scale acceleration-driven neutron facility. To this end, *ISIS*[7] is used as example, with an emphasis on those operational aspects of the facility which might be less familar to the target audience – e.g., a typical last-generation neutron spectrometer or the associated data analysis & mining infrastructure (the so-called 'tertiary' instrument). Pulsed neutron instrumentation is covered in some depth, including how it differs from the use of continuous sources, what are the primary components of a pulsed-neutron instrument, and what can be done to boost the useful neutron flux via the use of neutron-guide technology or multiplexing techniques.[27–34] These considerations serve to introduce a number of success criteria, from source power, reliability, and optimisation (clearly within the remit of the accelerator scientist & engineer) all the way down sample environment or to the nurturing of a strong user and stakeholder base associated with the facility. To illustrate the above, we present a series of case studies across contemporary global challenges, from energy research (gas storage and battery materials)[35–43] and chemical catalysis[44] to waste remediation and soil pollution.[45] Other relevant applications include the study of matter under extreme conditions of pressure and temperature relevant to the Earth Sciences,[46,47] exotic (quantum) phases of matter at high magnetic fields,[48] stress measurements of engineering components such as those found in gas-cooled nuclear reactors,[49] the optimisation of shampoo formulations and magnetic-recording media using small-angle neutron scattering and reflectometry,[50] the analysis of archeological artifacts,[51] and recent efforts by the semiconductor industry aimed at mitigating the detrimental effects of cosmic radiation on electronic devices.[52,53] The examples provided also serve to emphasize the need for the development of increasingly complex sample-environment equipment to emulate realistic conditions,[54] the use of complementary techniques alongside neutron studies,[55] and industrial applications.[56]

In the last section of this second lecture, we present a number of challenges and opportunities with a view to stimulating further work by early-career researchers in accelerator science and engineering. These include the optimisation of cold-neutron production at spallation sources, and materials and engineering challenges associated with the use of high-power proton accelerators. Further into the future, we explore the enticing possibility of combining accelerator and reactor technologies into a single neutron facility, an option which still needs to be explored in greater detail, as proposed recently in Ref. 57. We close by considering the use of inertial fusion for neutron production, a possibility that remains well beyond current technologies yet it most definitely sets a horizon for future and exciting developments beyond the imaginable at the present time.[58]

In closing this introduction, I thank Dr Graeme Burt from the *Cockcroft Institute of Accelerator Science & Technology* and Prof Ken Peach from the *The John Adams Institute for Accelerator Science* for their invitation to give these and previous lectures on the same topic at Daresbury Laboratory and the University of Oxford, respectively. I am also indebted to Dr John Thomason from the *ISIS Accelerator Division* and Prof Javier Bermejo from the *Consejo Superior de Investigaciones Científicas* for enjoyable and insightful discussions on the latest developments in accelerator technology in the context of neutron and condensed-matter science.

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2 John Adams Institute for Accelerator Science: `www.adams-institute.ac.uk`

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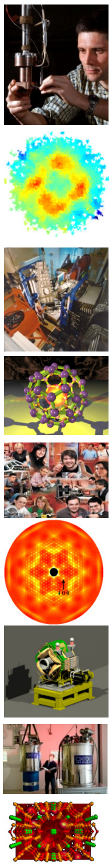

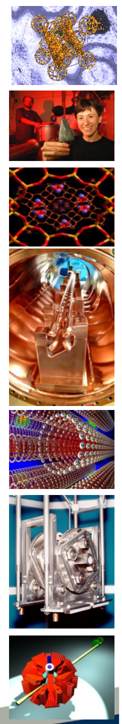

Accelerator-based Neutron Sources for Condensed Matter Research

Lecture I: Neutron Production

Felix Fernandez-Alonso

ISIS Pulsed Neutron & Muon Source
Rutherford Appleton Laboratory
Science and Technology Facilities Council

Applications of Accelerators
Cockcroft Institute Lecture Series
Winter Term 2015

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Outline

- Why neutrons are so special – a quick dive.
- Why we need accelerators.
- How accelerator-based neutron (and muon) sources work.

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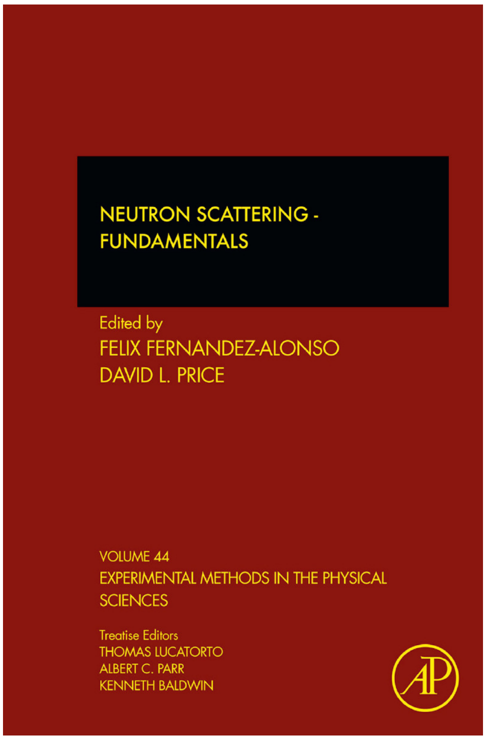
For Much More



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Why Are Neutrons So Special?

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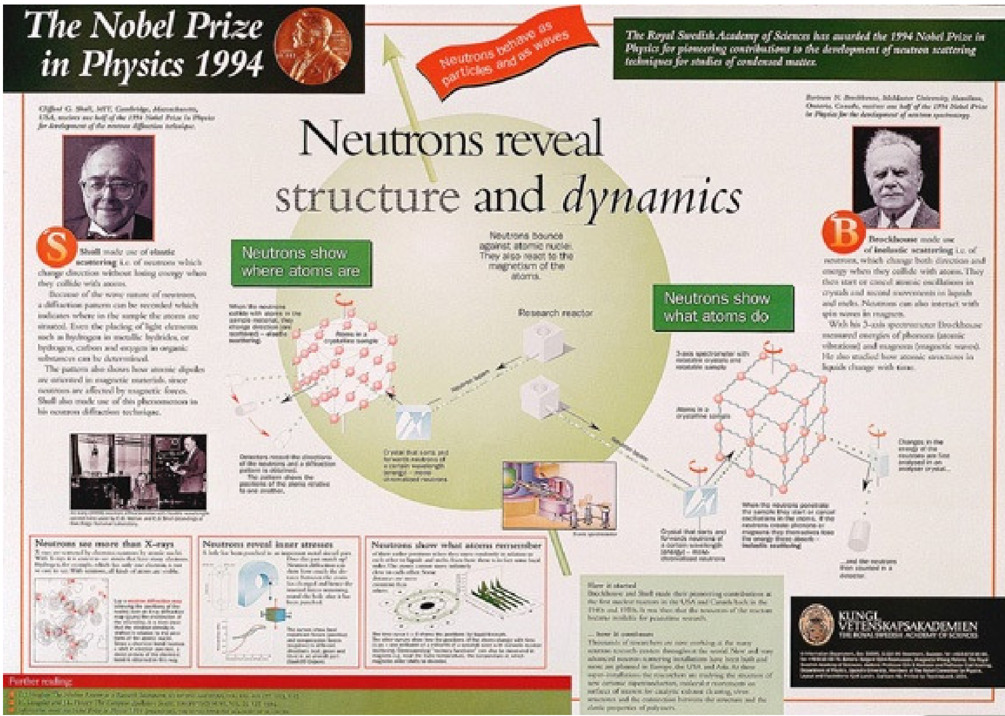
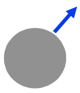
Neutron Science: Achievements



Neutrons can tell us ***where atoms are*** (structure)
and ***what atoms do*** (dynamics)

"Neutral Protons" as Condensed Matter Probes

Neutron		Photon	
– Mass	1 amu	– Rest mass	0 amu
– Spin	½	– Spin	1
– Charge	0	– Charge	0
– Interaction	Nuclear	– Interaction	E/B dipole …



Thermal Neutrons (T = 300 K)

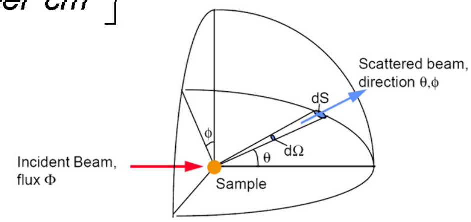
- Energies (meV) — motions in condensed matter (e.g., vibrations).
- Wavelengths (Å) — interatomic distances.
- Neutral particles — high penetration power.
- Nuclear interaction — δ-like (s-wave scattering).
- Spin — magnetic dipole moment ~1.9μ_N
- Stable — lifetime ~15 min

Hard to produce & manipulate

Basic Observables: Scattering Cross Sections

Given an incident beam: $\Phi = \left[\textit{incident neutrons per cm}^2 \right]$

This is what we can measure:



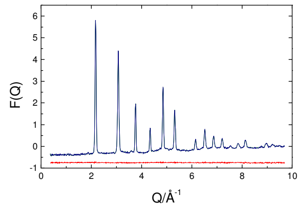
Cross sections also depend on polarisation of incident & scattered neutron.

(1) Transmission experiment:

$$\sigma = \frac{\left[\textit{scattered neutrons}\right]}{\Phi}$$

(2) Diffraction experiment:

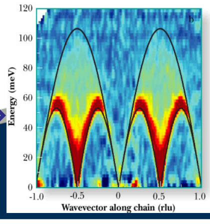
$$\frac{\partial\sigma}{\partial\Omega} = \frac{\left[\textit{scattered neutrons} \text{ into } \partial\Omega\right]}{\Phi\,\partial\Omega}$$



Diffraction pattern (crystallography)

(3) Spectroscopy experiment:

$$\frac{\partial\sigma}{\partial\Omega\partial E} = \frac{\left[\textit{scattered neutrons} \text{ into } \partial\Omega \,\&\, \partial E\right]}{\Phi\,\partial\Omega\partial E}$$



"Dynamic" Diffraction pattern

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A Health Warning on Jargon

What We Mean by "Elastic" and "Inelastic" Scattering

- Thermal neutrons (meV energies) can only exchange kinetic energy with target (unless they undergo nuclear absorption).

- Strictly speaking, thermal neutrons can only undergo elastic (s-wave) scattering in the scattering (centre-of-mass) frame.

- The condensed-matter scientist always refers to scattering in the laboratory frame (typically with target at rest).

- In lab frame, two types of thermal neutron scattering:
  - "Elastic": velocity of neutron does not change.
  - "Inelastic": velocity of neutron changes due to atomic motions (a Doppler shift).

Keep this in mind, to avoid confusion

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The Double Differential Cross Section

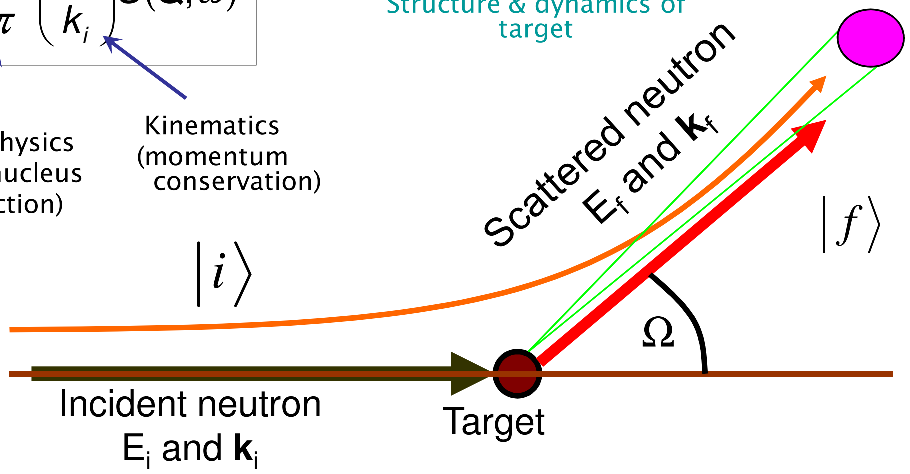
$$\frac{d^2\sigma}{d\Omega dE} = \frac{\sigma_{TOT}}{4\pi}\left(\frac{k_f}{k_i}\right)S(\mathbf{Q},\omega)$$

This is what the neutron scientist wants. Structure & dynamics of target

This is what you measure

Nuclear physics (neutron-nucleus cross section)

Kinematics (momentum conservation)



Energy and Momentum Exchange with Target

$$\hbar\omega = (E_i - E_f) = \frac{\hbar}{2m}\left(\mathbf{k}_i^2 - \mathbf{k}_f^2\right)$$

$$\mathbf{Q} = \left(\mathbf{k}_i - \mathbf{k}_f\right)$$

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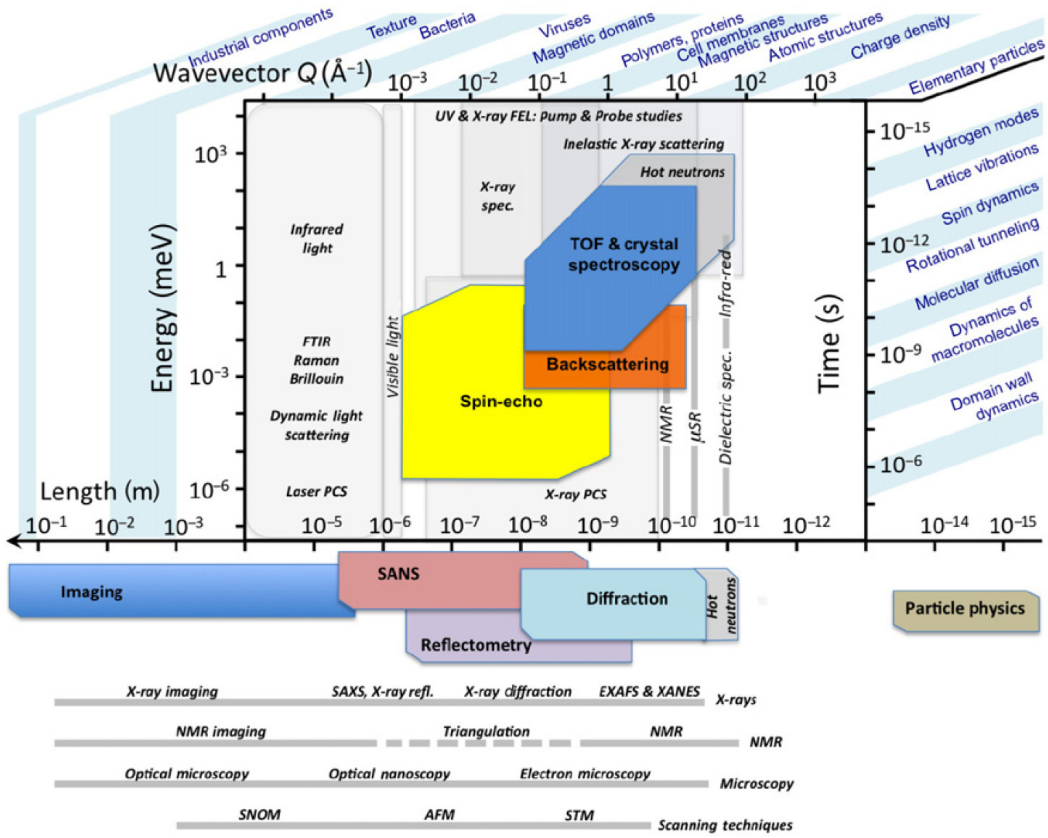
Where Atoms **Are** and **Do**: Neutrons



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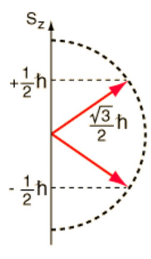
Thermal Neutron Scattering is All about Spin

A few ground rules

S=½



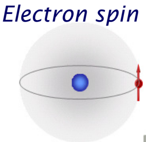
Nuclear spin

- Neutrons, atomic nuclei, and electrons all have intrinsic spin.
- Neutron scattering cross sections are spin dependent.
- Nuclear scattering:
  - Spin-flip → incoherent scattering → single-particle properties (number density, vibrations, diffusion).
  - No spin flip → coherent scattering → two-body correlations (lattice structure, phonons).

  By definition, zero-spin nuclei will only scatter coherently (e.g., C,O)
- Magnetic (electron) scattering: magnetic-dipole interaction.
- We can also polarise (align) spins in sample and alter contrast.

Consequences

Electron spin (S=½)



- Polarisation analysis allows separation of coherent/incoherent or nuclear/magnetic scattering → very convenient and very powerful.
- Precession of neutron spin in magnetic fields can be used as a clock in order to measure its velocity very precisely (interferometrically): neutron-spin-echo techniques.

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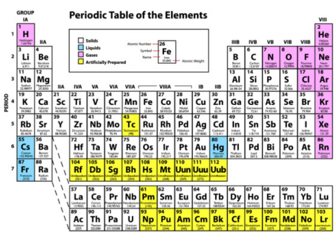
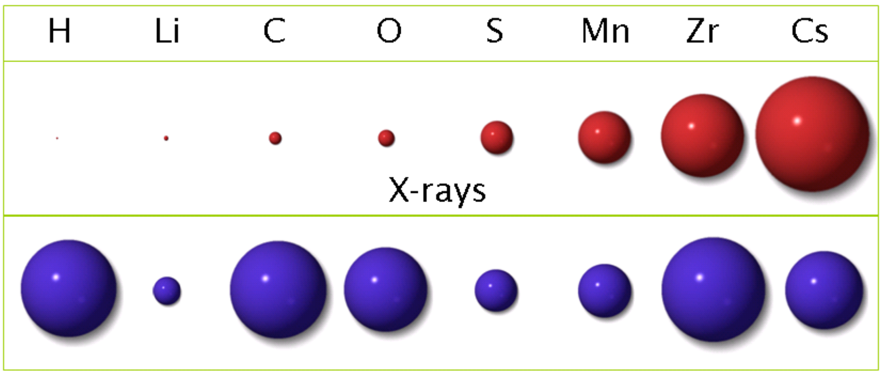
The Periodic Table: X-rays vs. Neutrons

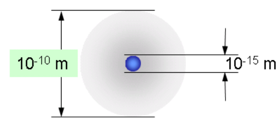
- X-rays: see electron clouds.
- Neutrons: see the atomic nucleus.





Neutrons

Nuclear scattering



- Hydrogen: large cross section, largely invisible to X-rays.
- Different nuclear isotopes can have very different neutron cross sections.

Isotopes: what do we gain?

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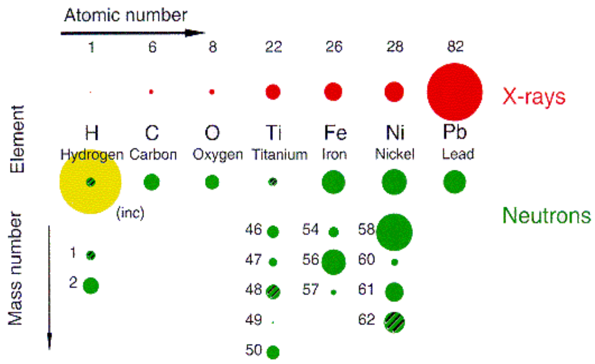
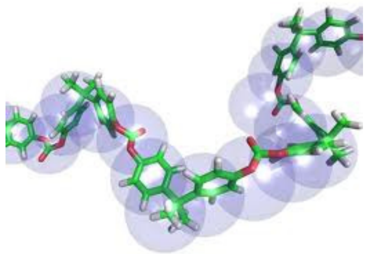
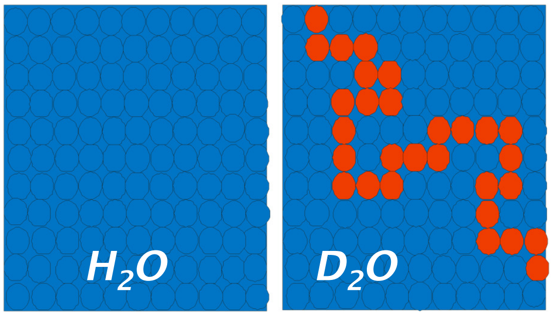
Constrast Variation: The Added Dimension



The diameters of the circles shown scale with the scattering amplitude f_x ($\sin\theta = 0$) for x-rays, and b_{coh} * 10 for neutrons. Hatching indicates negative scattering amplitudes.



A polymer (mostly H) in water …



Where ??? *There !!!*

- H/D substitution is at the heart of many neutron experiments.
- Hydrogen: central to biology, organic chemistry, soft matter, aqueous chemistry, energy, catalysis …
- Same principle applies to all elements (if you can get the isotope!)

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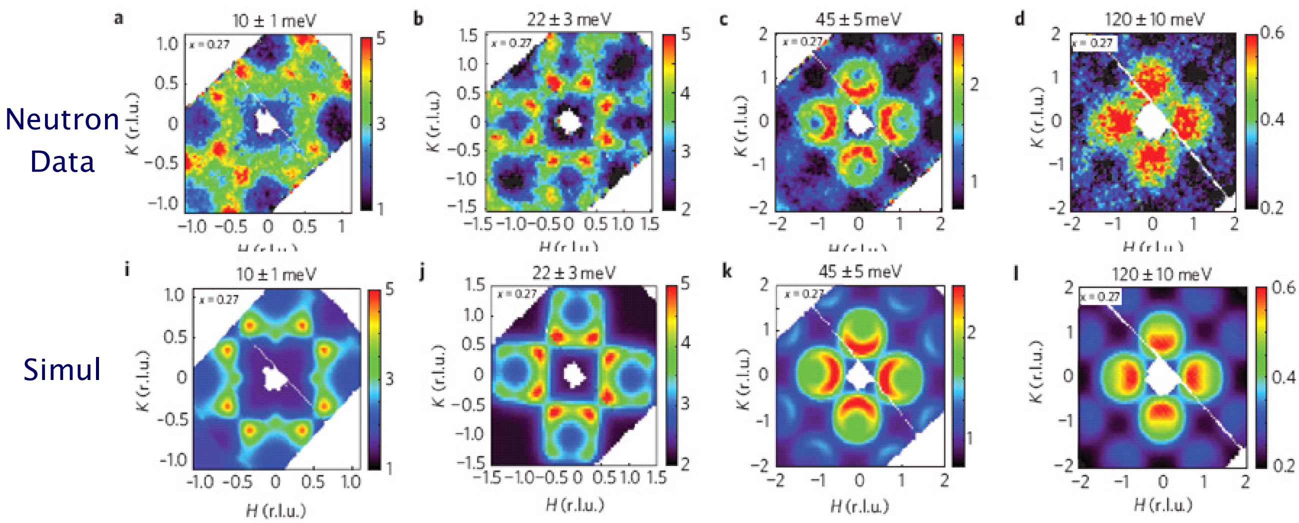
Magnetic Scattering: No Neutrons, No Insight

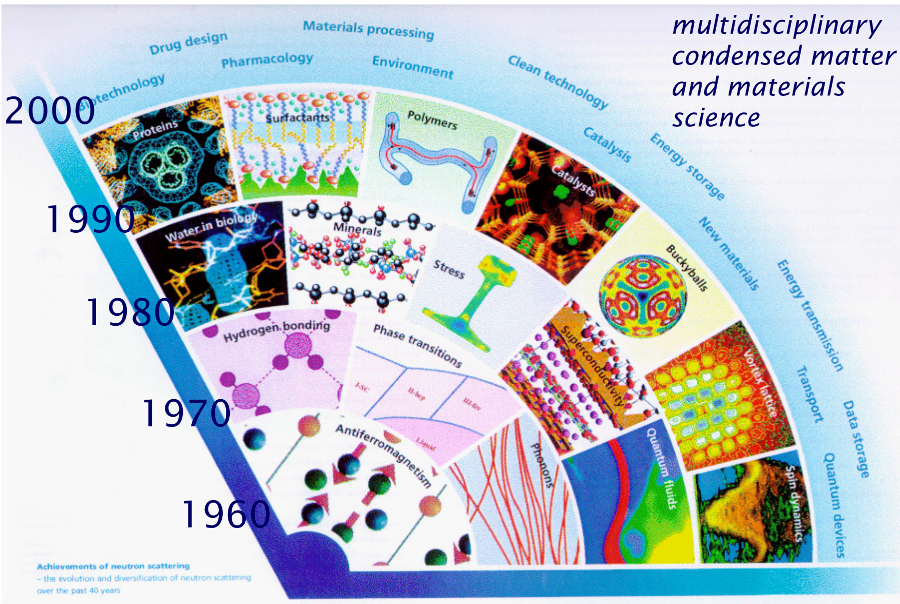


Iron-based superconductor $Fe_{1.04}Te_{0.73}Se_{0.27}$

Nature Physics 5 555 (2009)

.

One Probe, Many Questions



Particularly to study hydrogen-containing materials and magnetism.

More examples later …

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Why Accelerators?

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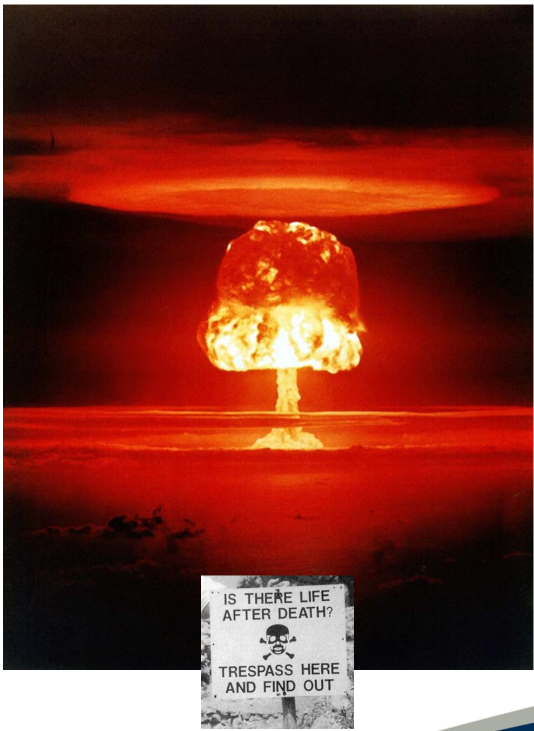
The Quick-and-dirty Way to Produce Neutrons



Not a wise option

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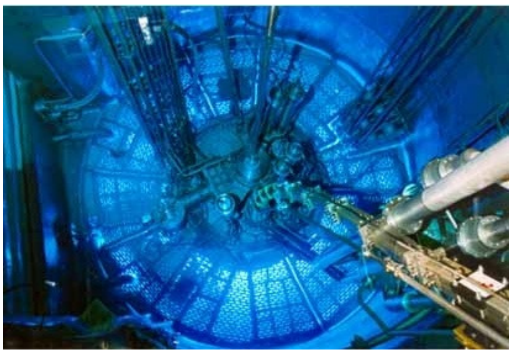
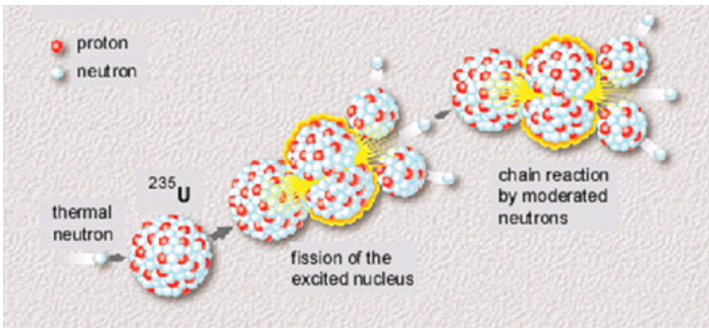
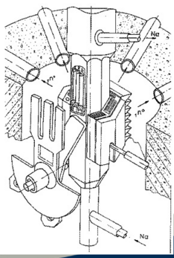
A Safer Option: The Nuclear Reactor

ILL Reactor, France
(58 MW)



(Controlled!) Nuclear Fission





- Requires fissile material (e.g., Uranium).
- Chain reaction.
- Continuous operation – exception: IFR pulsed (!) reactor in Dubna, Russia (2MW/1.5GW average/peak power).

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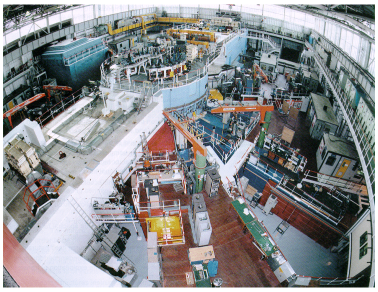
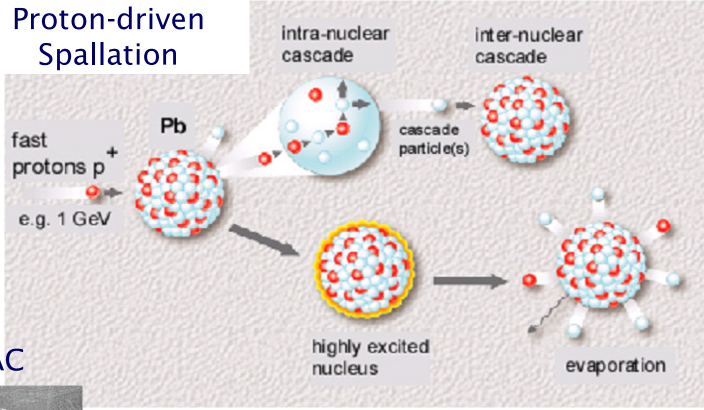
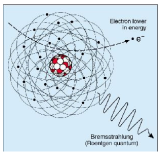
An Even Safer (and cleaner) Option: A Particle Accelerator

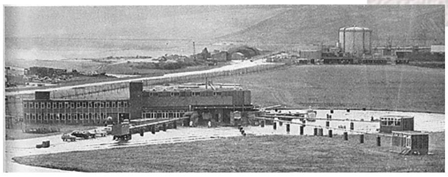
ISIS Facility, United Kingdom
(operational since 1984)





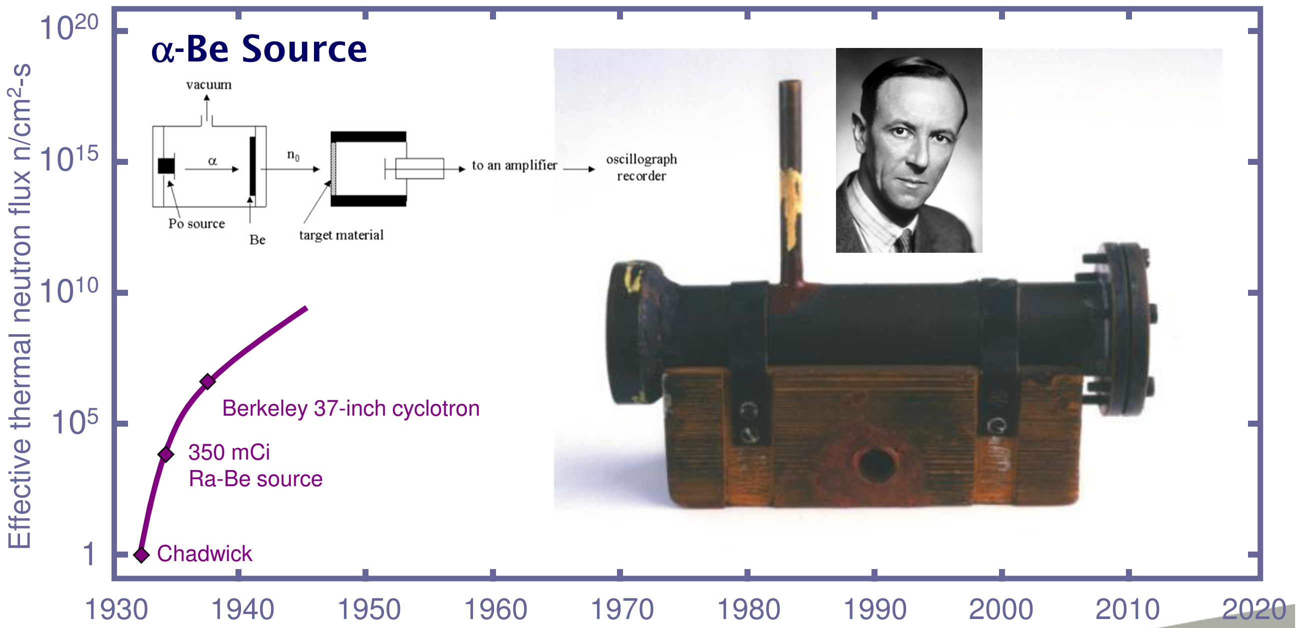
Its predecessor: the Harwell e-LINAC





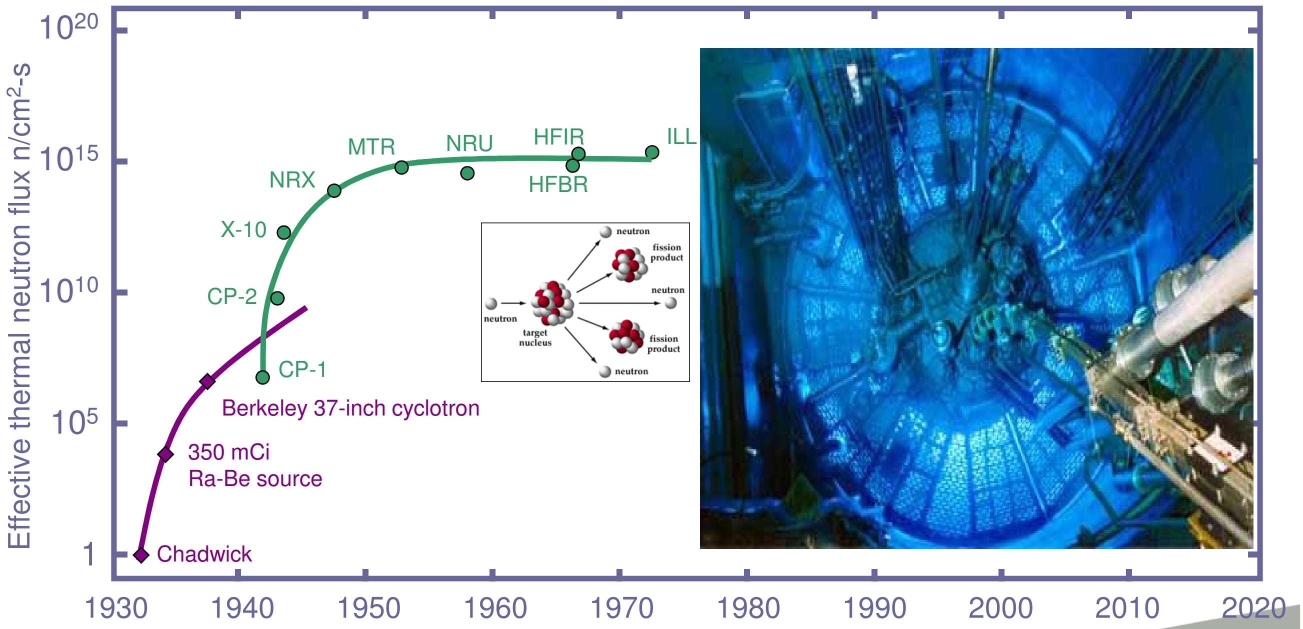
- A fast particle, normally a proton, chips or 'spalls' nucleons from a nucleus.
- There is no chain reaction.
- Neutrons are produced with MeV energies.

Historical Evolution of Neutron Sources



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

Historical Evolution of Neutron Sources



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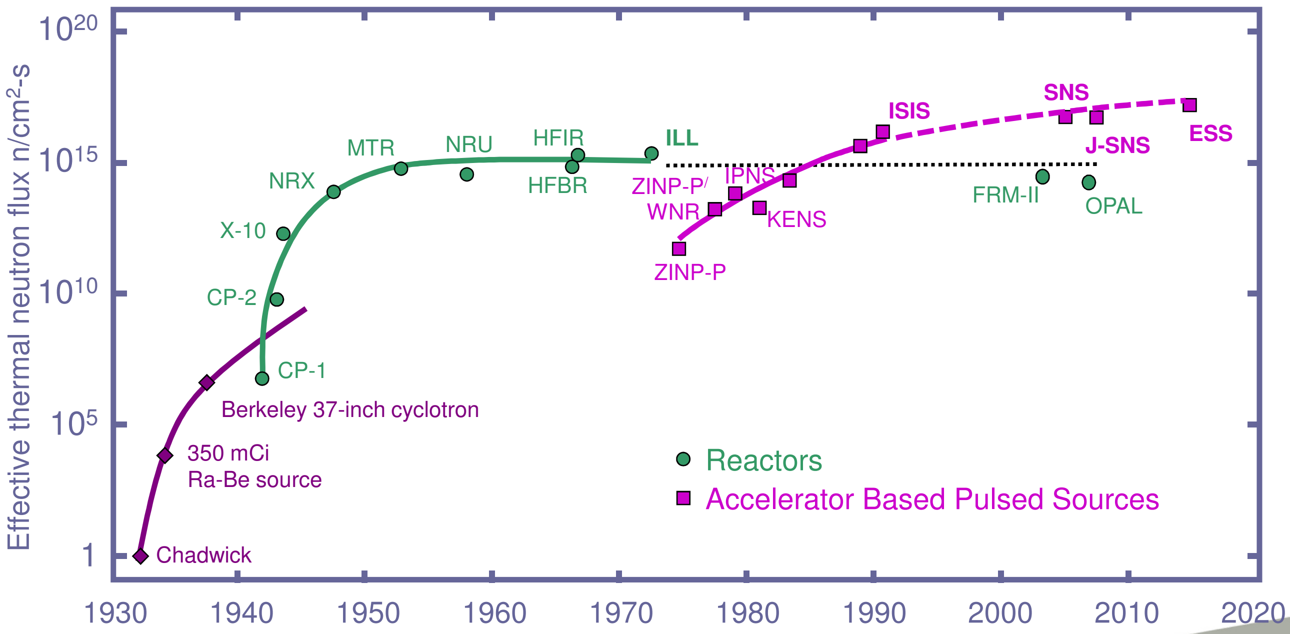
Historical Evolution of Neutron Sources



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

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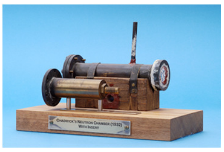
Reactor vs Accelerator-based Neutron Sources

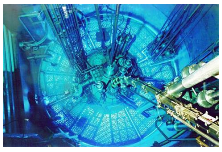
Reactor-based source:

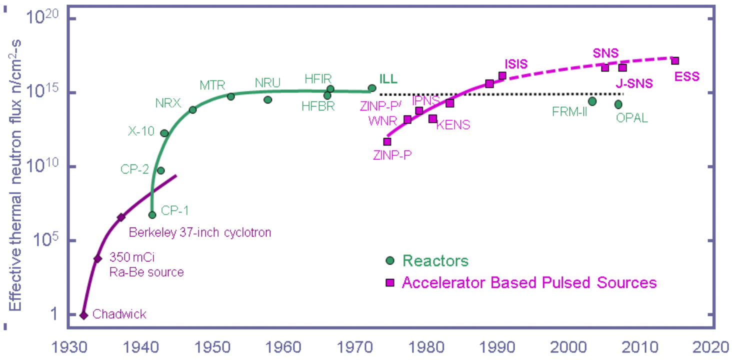
- Neutrons produced by fission reactions
- Continuous neutron beam
- 1 neutron/fission .

Accelerator-based source:

- Neutrons produced by spallation reaction
- 10s of neutrons/proton
- Neutrons are pulsed, follow proton beam time structure.
- A pulsed beam with precise t_0 allows neutron energy measurement via TOF ($v=d/t$)







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

Accelerator based-sources have not yet reached their limit and hold out the promise of higher intensities.

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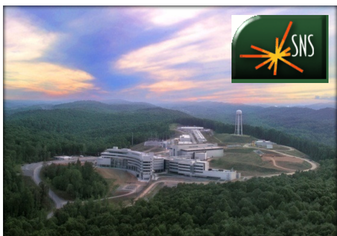
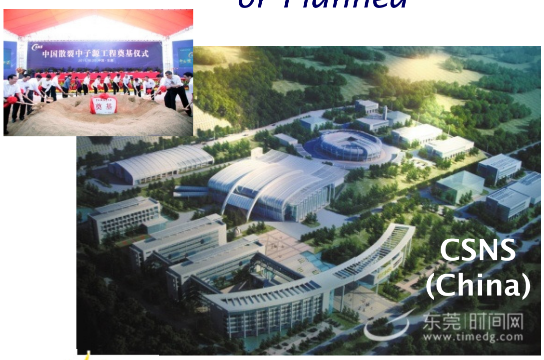
The Golden Age of Spallation Neutron Sources

Operational



Under Construction or Planned



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How Spallation Neutron (and Muon) Sources Work

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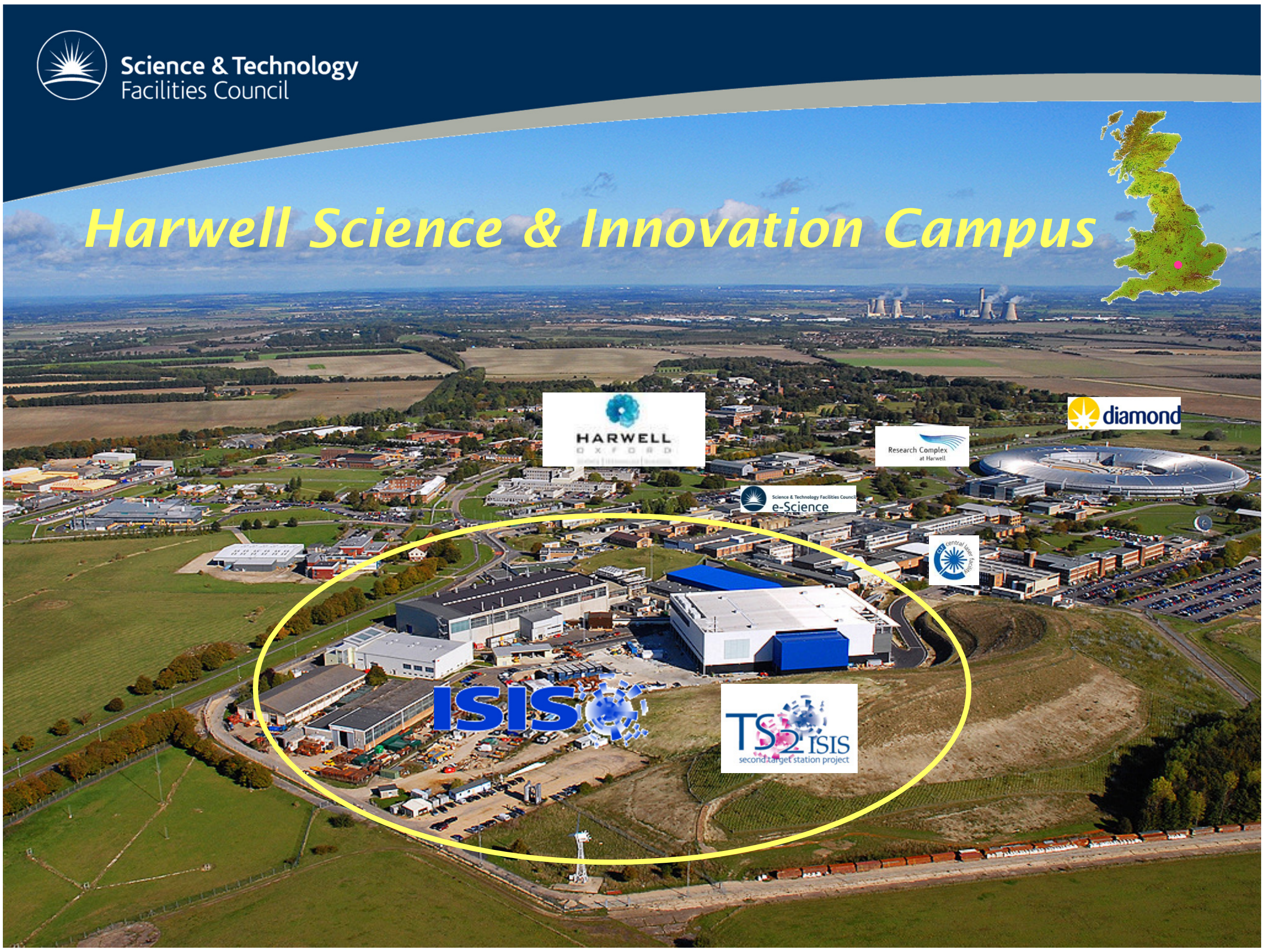
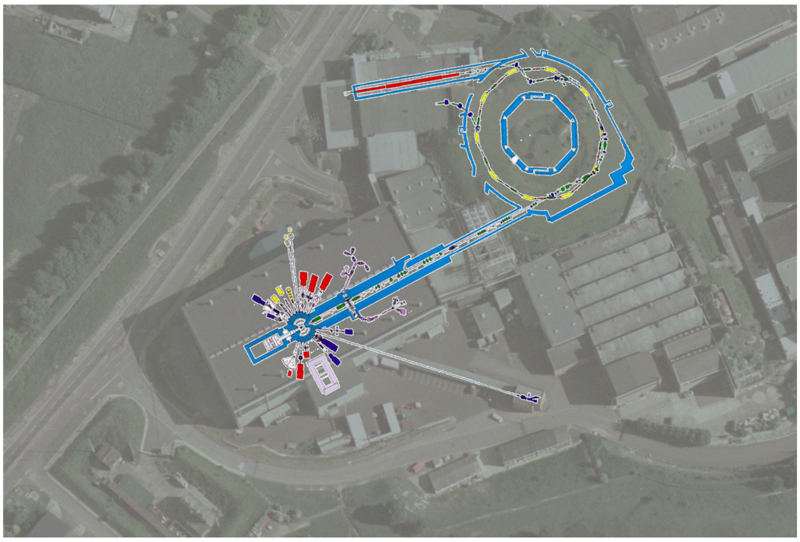


ISIS Target Station I



Formerly NIMROD (particle physics)

200 μamp proton beam at 800 MeV hitting heavy-metal target (50 Hz rep rate, 200 kW).

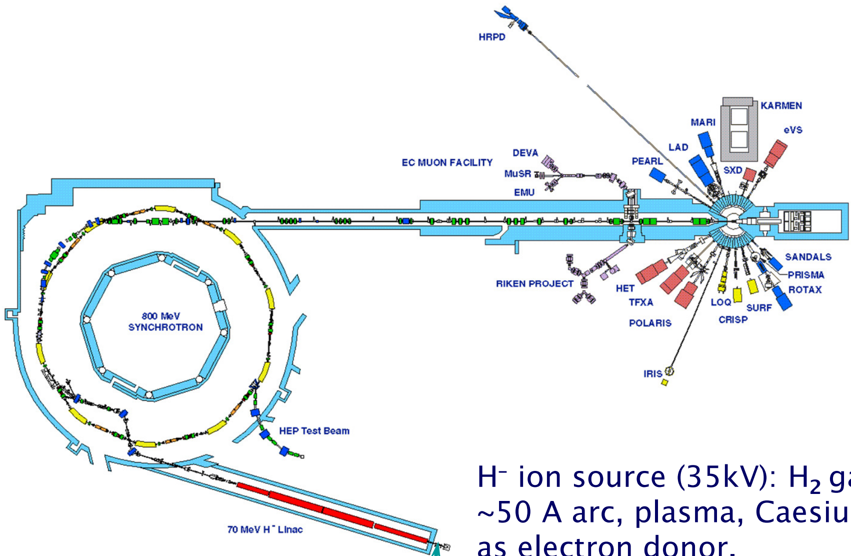
1984
(30 years Dec 2014)

Protons are used to produce $>10^{16}$ n/s.

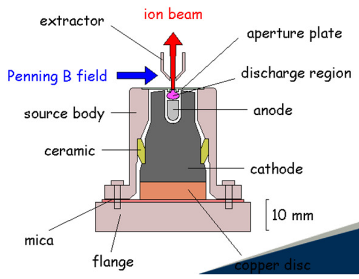
Neutron pulses are short (μsec).

How many neutrons produced since 1984?

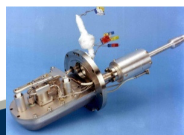
Neutrons from Spallation: The Ion Source

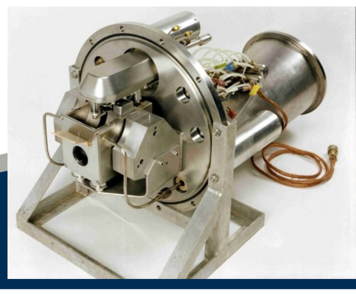


H^- ion source (35kV): H_2 gas, ~50 A arc, plasma, Caesium as electron donor.

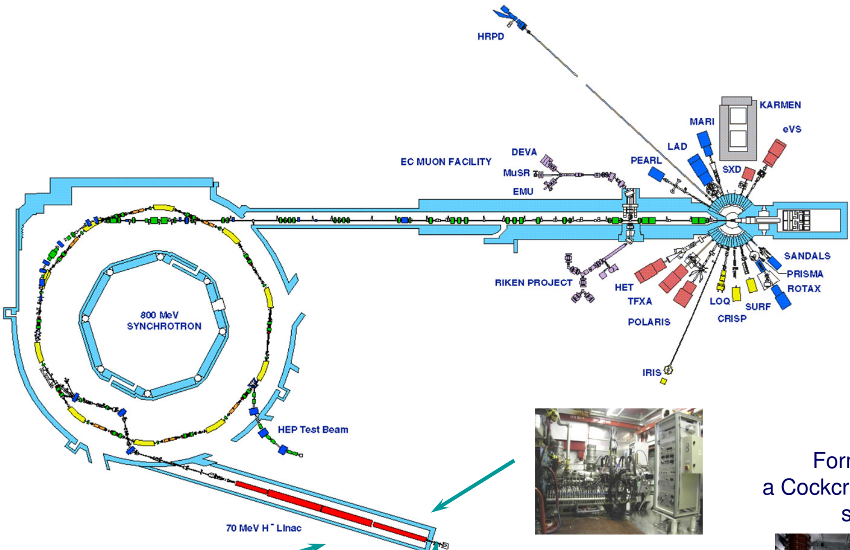


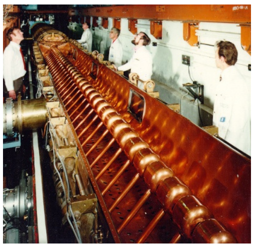
H^- ion source





Neutrons from Spallation: RFQ & LINAC





H^- ions accelerated to 70MeV in LINAC

RFQ: H^-, 665 keV, LINAC injection

Formerly a Cockcroft-Walton set

H^- ion source

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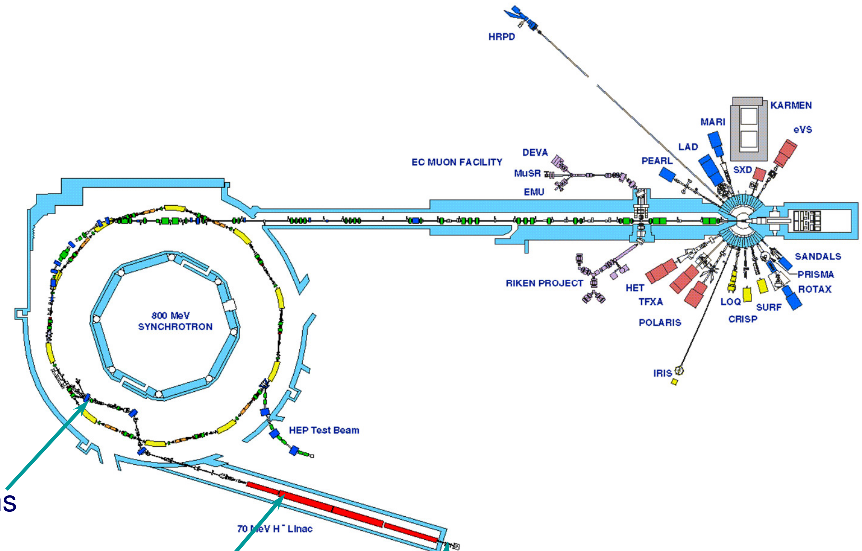
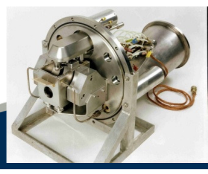
Neutrons from Spallation: Charge Stripping

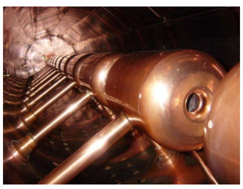
Al_2O_3 , 0.25 μm
Creation of p^+ and injection into synchrotron

Stripped of electrons
$H^- \Rightarrow p^+$



H^- ion source





H^- ions accelerated to 70MeV in LINAC

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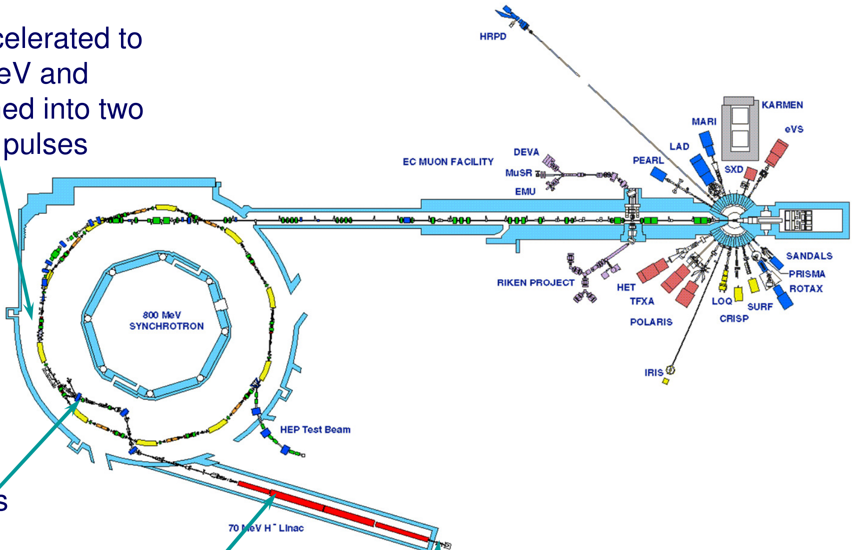
Neutrons from Spallation: Synchrotron

p^+ accelerated to 800MeV and bunched into two 0.3µs pulses



Stripped of electrons
H^- ⇨ p^+

H⁻ ion source

H⁻ ions accelerated to 70MeV in LINAC

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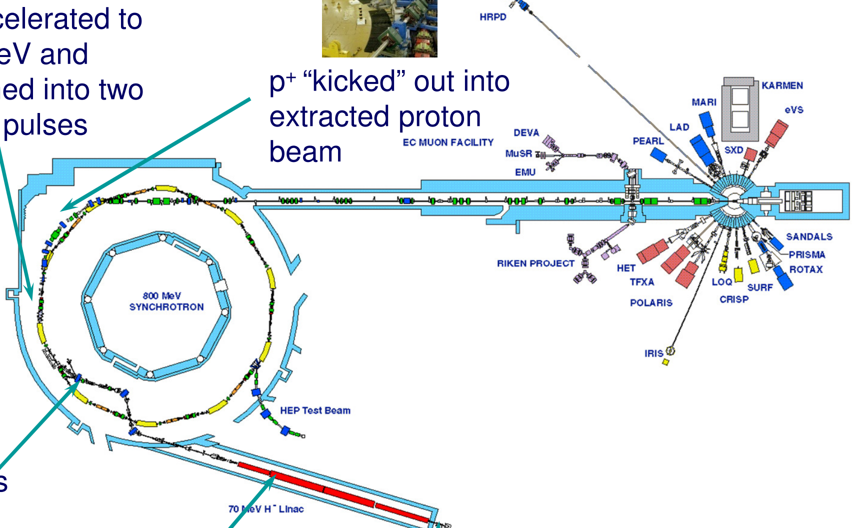
Neutrons from Spallation: Beam Extraction

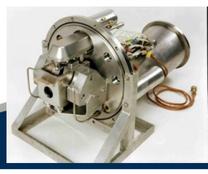
p^+ accelerated to 800MeV and bunched into two 0.3µs pulses

p^+ "kicked" out into extracted proton beam

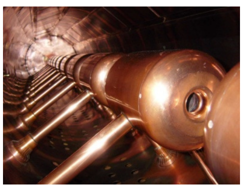


Stripped of electrons
H^- ⇨ p^+

H⁻ ion source



H⁻ ions accelerated to 70MeV in LINAC



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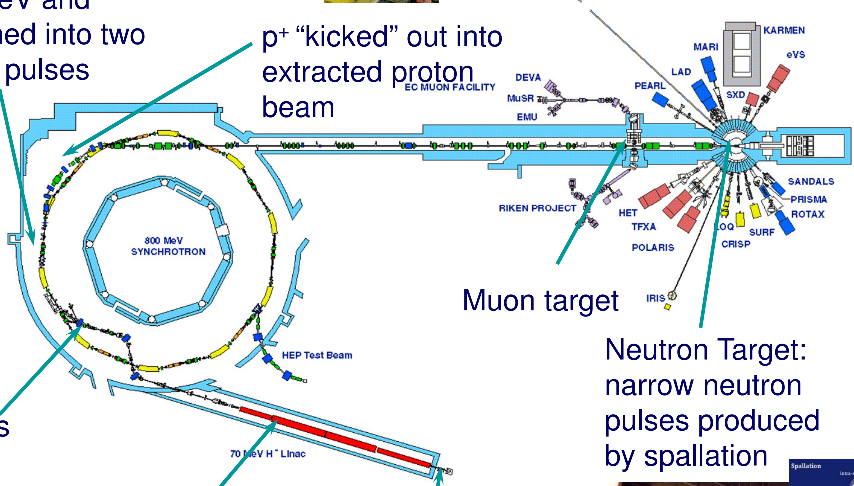
Neutrons from Spallation: Muon and Neutron Production

p^+ accelerated to 800MeV and bunched into two 0.3µs pulses

p^+ "kicked" out into extracted proton beam

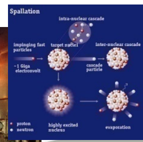


Stripped of electrons

$H^- \Rightarrow p^+$

Muon target

Neutron Target: narrow neutron pulses produced by spallation



H^- ions accelerated to 70MeV in LINAC

H^- ion source

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Extracted Proton Beam

Frequency of extraction determines source repetition frequency (50Hz)
4/5 into TS1, 1/5 into TS2

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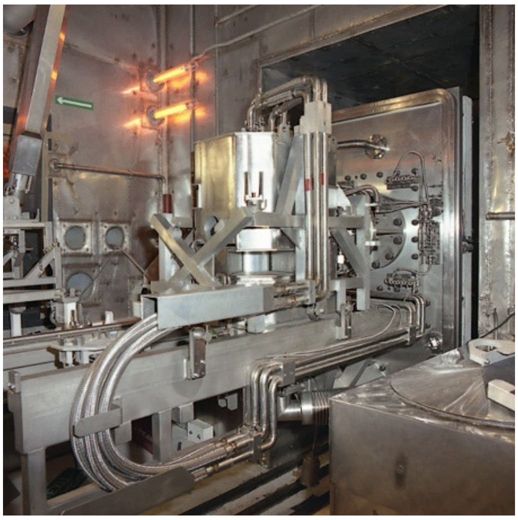
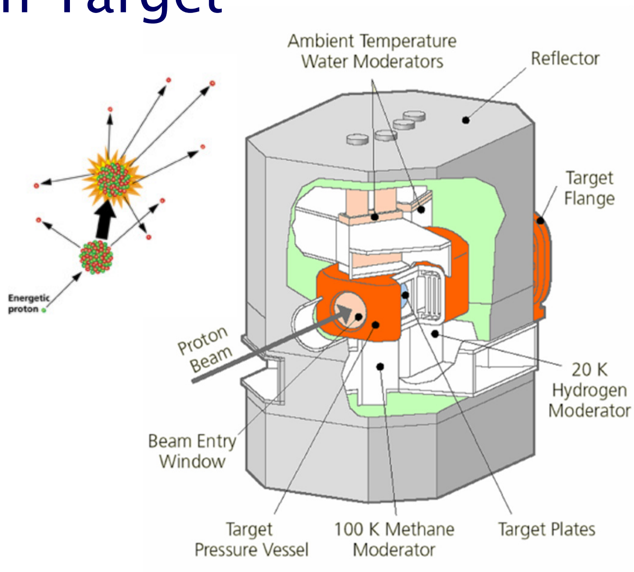
Spallation Target

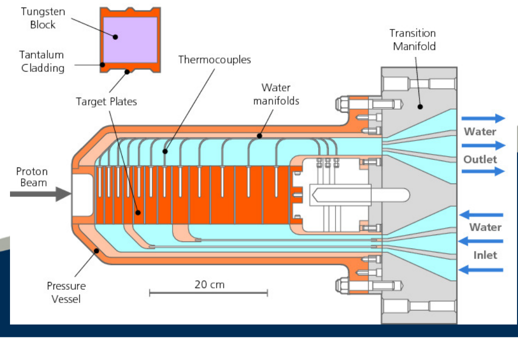




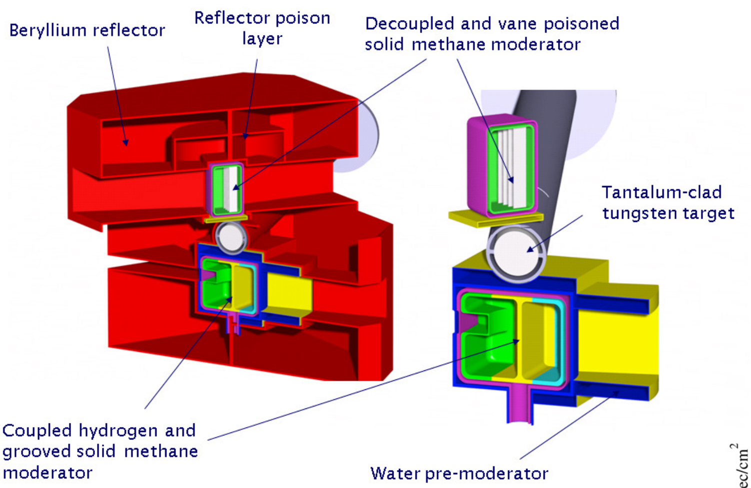
~2.5×10^{13} protons per pulse onto tungsten target (50 pps)

~15–20 neutrons / proton, ~4×10^{14} neutrons / pulse

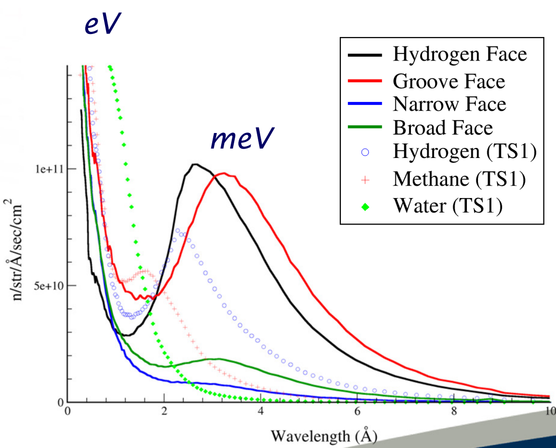
Primary neutrons from spallation: evaporation spectrum (E ~1 MeV, still not useful).



Neutron Moderation: From "M" to "m" eV



- Elastic nuclear scattering in a hydrogenous material.
- Temperature determines position of moderated "hump."



- Three moderators: liquid hydrogen (20 K), methane (100 K), water (315 K).
- Moderation is incomplete, to preserve time structure of pulse (μsec).
- Number of collisions needed about 10-20.
- Quite inefficient (1/10000 are useful)

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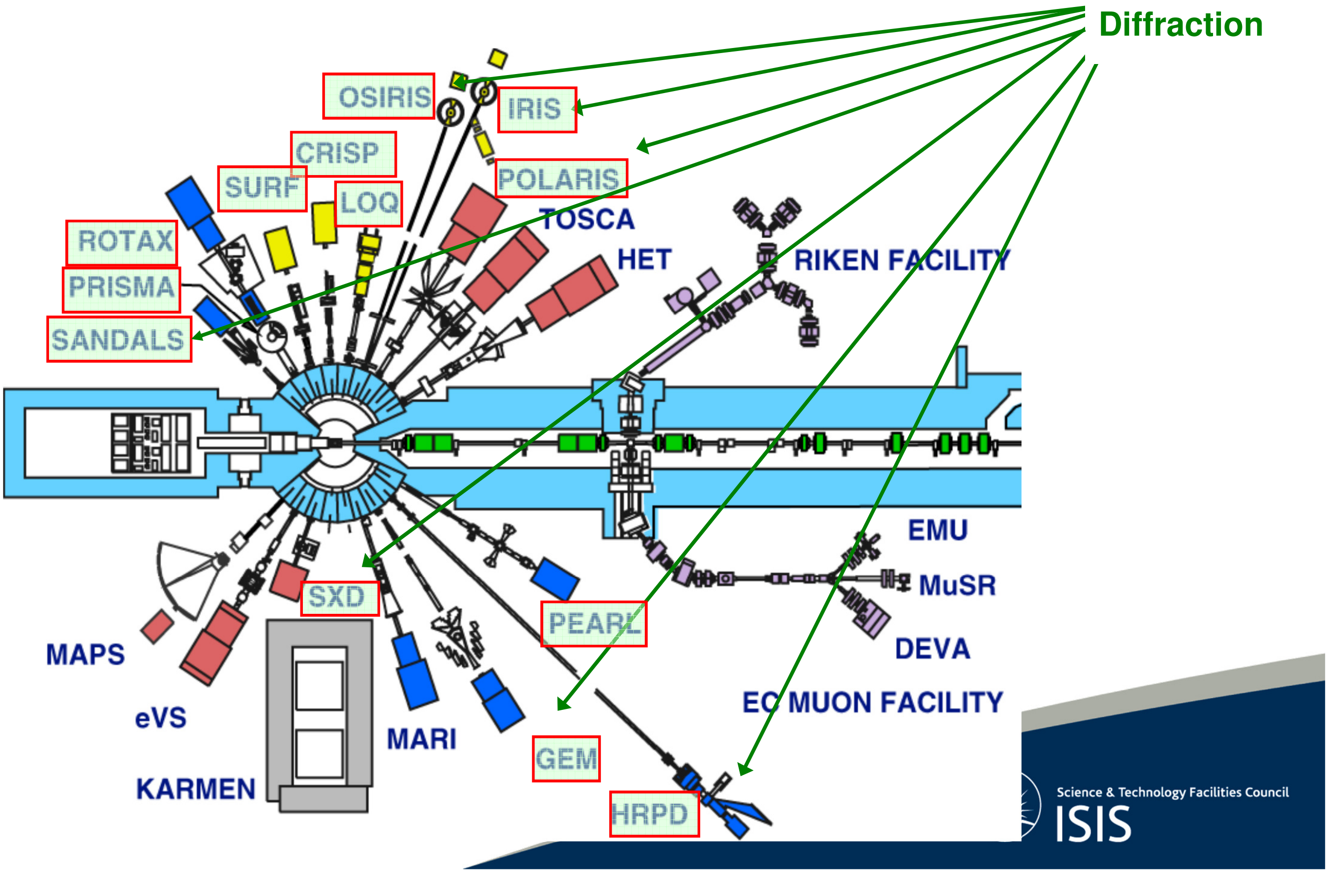
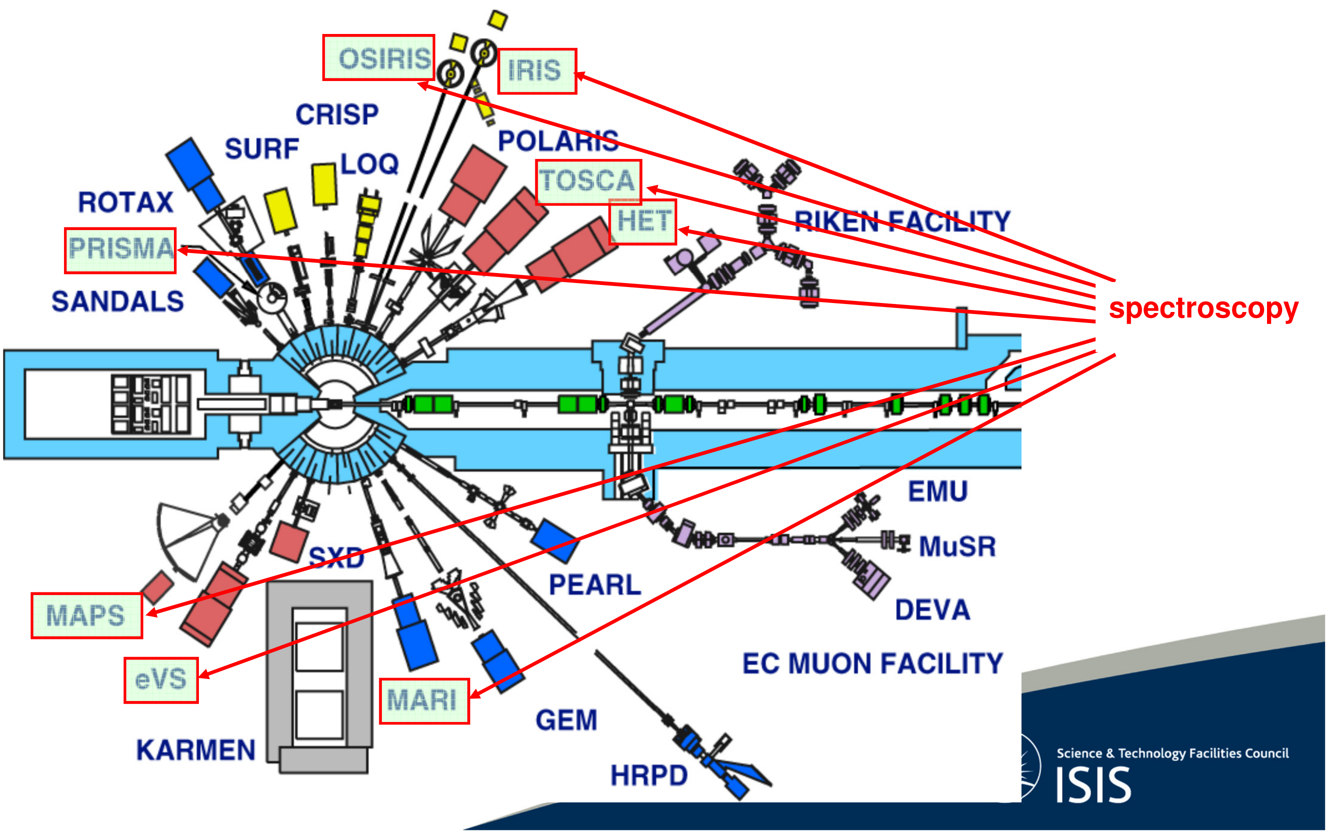
ISIS Neutron Instruments: Where Atoms Are (Structure)

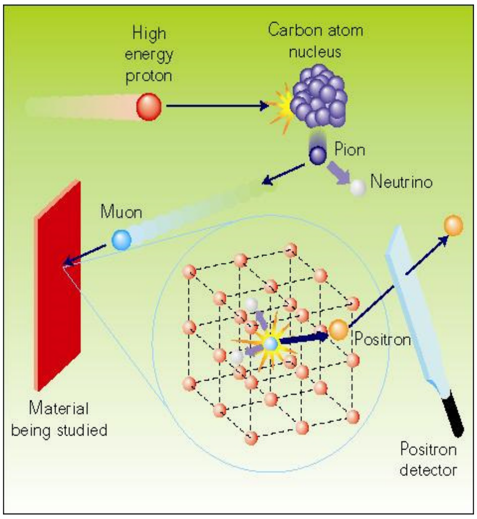


ISIS Neutron Instruments: What Atoms Do (Dynamics)

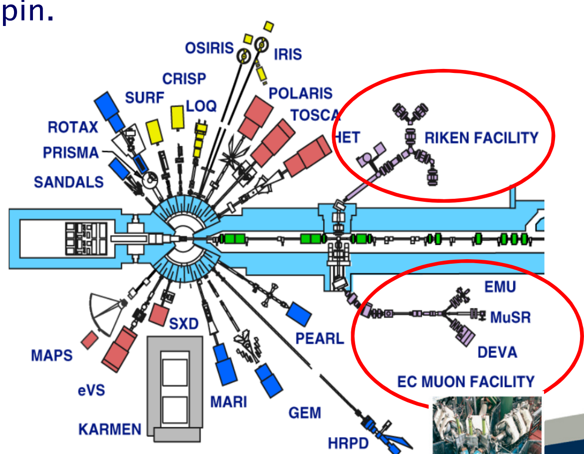


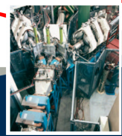
Brief Detour: ISIS Muons

Courtesy of AD Hillier (ISIS)



- High-energy protons collide with carbon nuclei producing pions.
- Pions decay into spin-polarised muons: $\pi^+ \rightarrow \mu^+ + \nu_\mu$
- Muons decay in 2.2μs: $\mu^+ \rightarrow e^+ + \nu_e + \nu_\mu$
- Positrons are emitted preferentially along direction of muon spin.





Muons are used as:

- Local magnetic probes (physics).
- Ultralight protons (chemistry).
- A source of neutrinos (MICE experiment).

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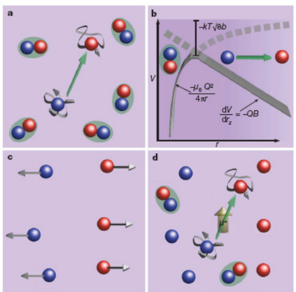
Brief Detour: Whetting Your Appetite for Muons

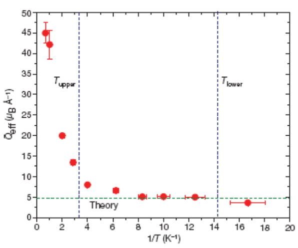
"Magneticitry"



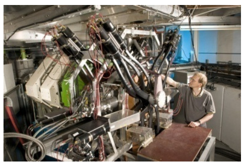
Emergent magnetic monopoles in "spin ices"

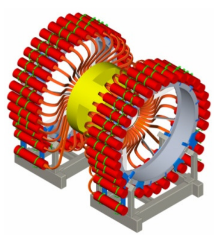
Nature ***461*** *956 (2009)*

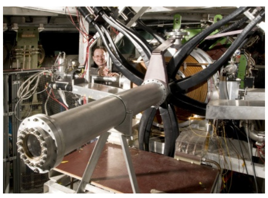
Muons give the effective charge of these quasiparticles

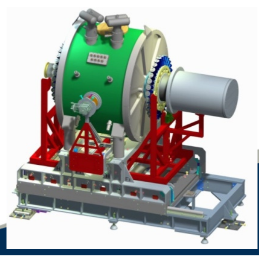


This is the subject of an entirely separate talk!

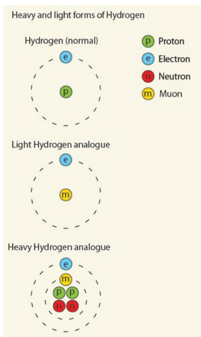






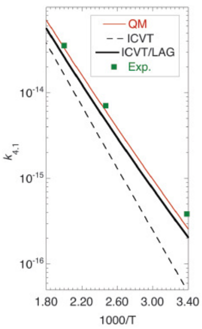


Muonium Chemistry



The H+H_2 reaction: the "quark" of chemistry.

Use of muons as an ultralight hydrogen atom to benchmark our understanding of chemical reactivity.



Science ***331*** 448 (2011)

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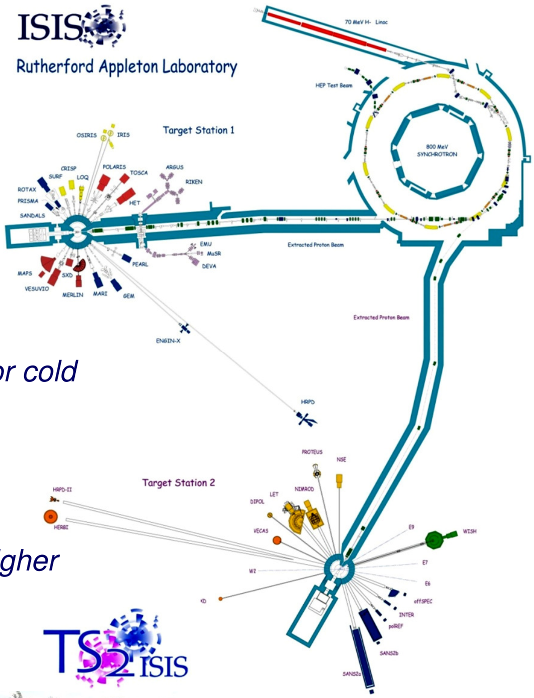
ISIS Target Station II

Takes one proton pulse out of five (10 Hz, 40 kW)

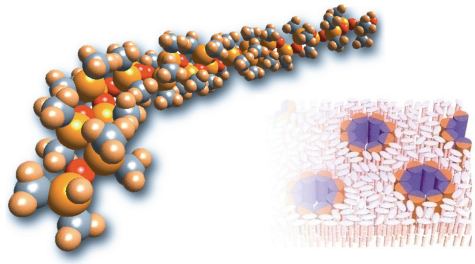
Aimed to meet scientific needs in key areas:

- Soft Matter
- Advanced Materials
- Bio-molecular Science
- Nanoscience



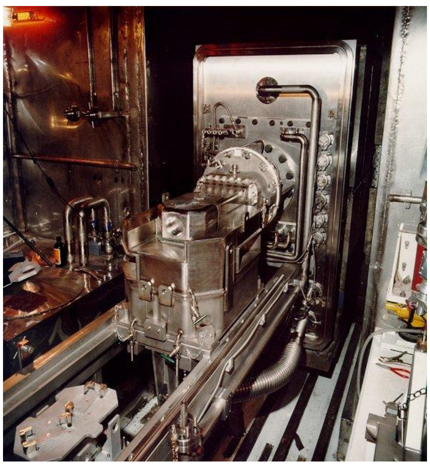
Optimised for cold neutrons.

Neutronic performance higher than TS1 with 1/5 power.

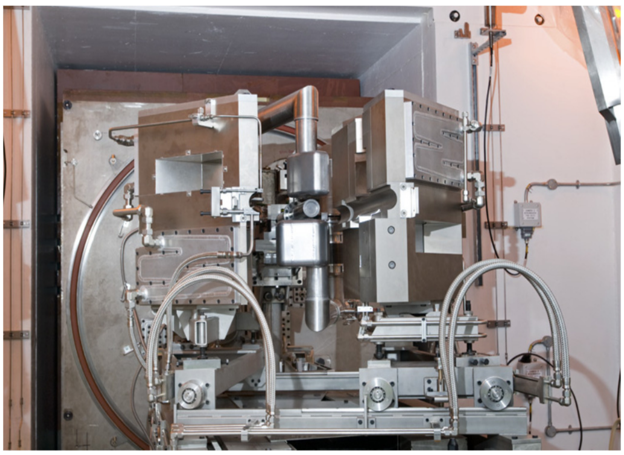


2008

Target Station II: Capitalising on Decades of Experience



1984



2007

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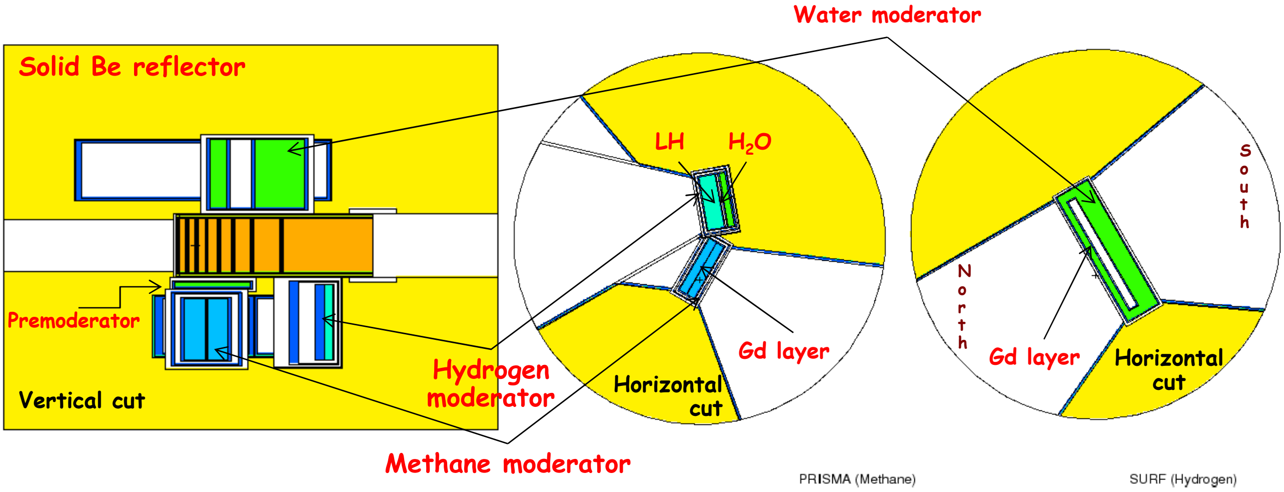
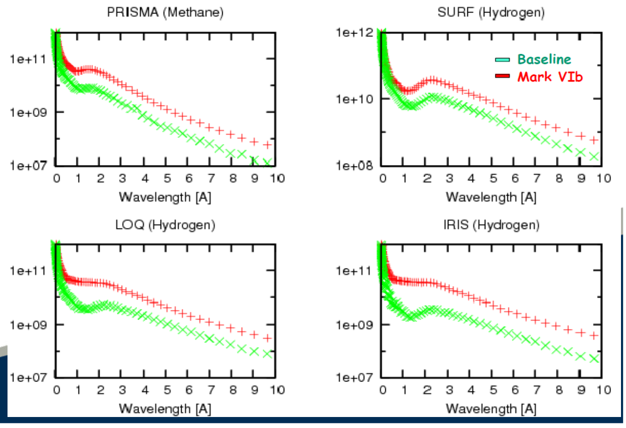
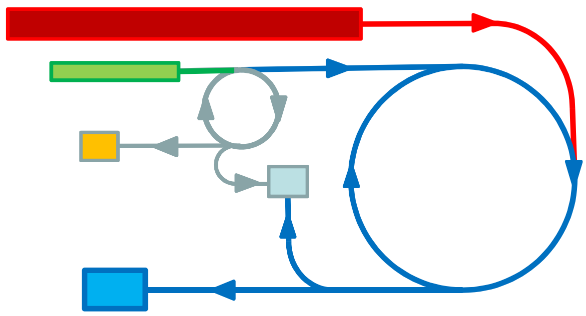
TS-I Target Upgrade

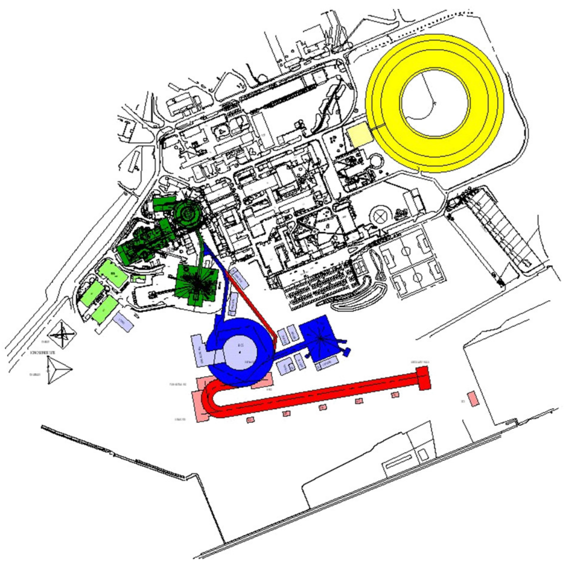


Feasibility phase in progress.



Accelerator Upgrade Paths at ISIS





0) Linac and TS-1 refurbishment

1) Linac upgrade, 180 MeV, ~0.5 MW

2) ~3 GeV booster synchrotron: MW target

3) 800 MeV direct injection: 2-5 MW target

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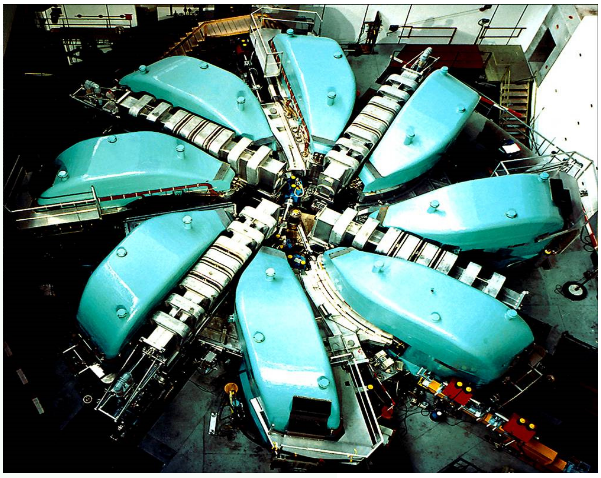
Other Large-Scale Facilities: SINQ at PSI

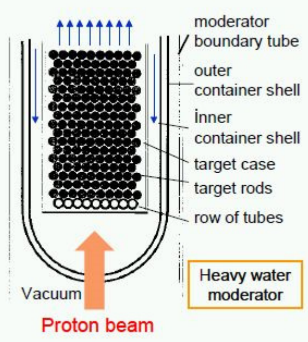


Operating since 1990s in Switzerland.

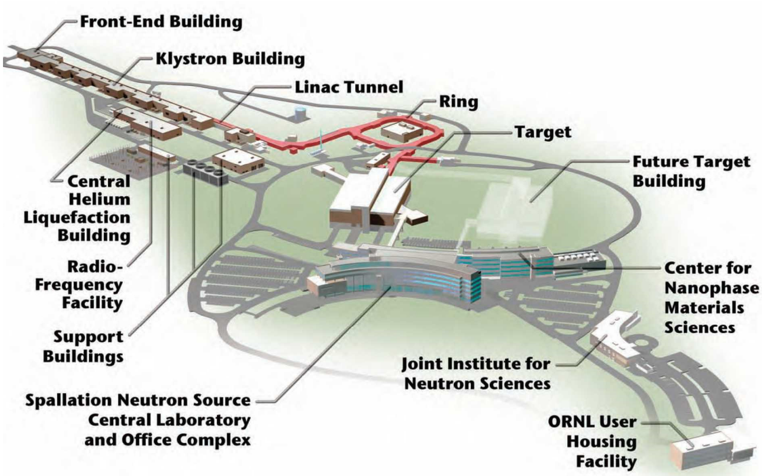
Proton cyclotron

590 MeV, 2 mA, 1.2 MW

The exception: continuous neutron beams (reactor-like).



Other Large-scale Facilities: SNS at Oak Ridge



Operational in USA since 2005

ISIS 'bigger sister'

LINAC (350m) + ring (250 m)

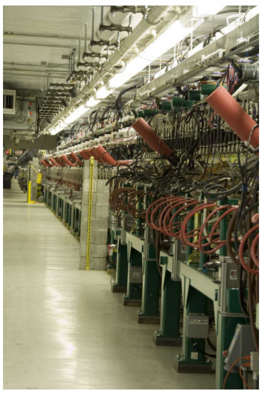
1 GeV H^- superconducting LINAC 185 MeV (first of its kind).

Compressor ring to achieve tight 700 ns pulses.

Liquid Hg target.

Currently operating at 1.4 MW

Second Target (ISIS-like) planned



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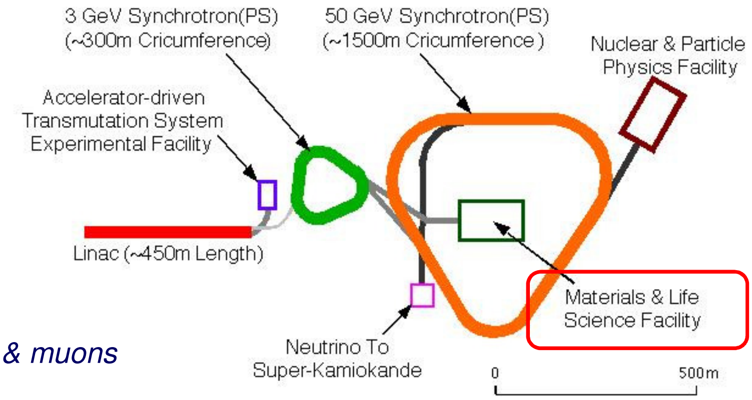
Other Large-scale Facilities: MLF at J-PARC



Liquid Hg target

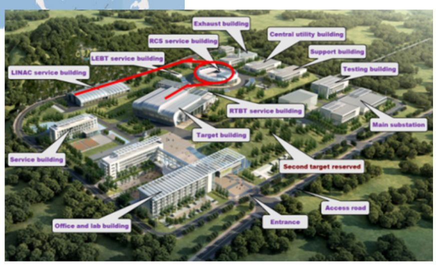
Neutrons & muons

Short-pulse like ISIS and SNS

High Intensity Proton Accelerator Project

1 MW+

Under Construction: CSNS in China

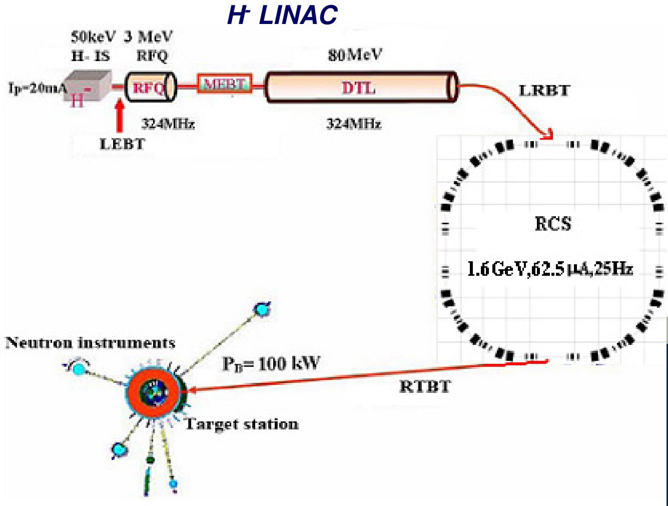


Very similar conceptually to ISIS

100 kW at 25 Hz, upgradable to 500 kW

Construction started 2011, aiming for completion early 2018.

H⁻ LINAC



Under Construction: European Spallation Source (ESS)

Pan-European effort led by Sweden & Denmark.

Projected costs of 1.8 G€ (10% UK).

Under construction – first neutrons expected 2019.

“Long pulse” (2.8 ms) – optimised for cold-neutron production, departure from ISIS-like source (“short pulse”).

2 GeV LINAC (602 m)

62.5 mA, 14 Hz, 5/125 MW average/peak power.

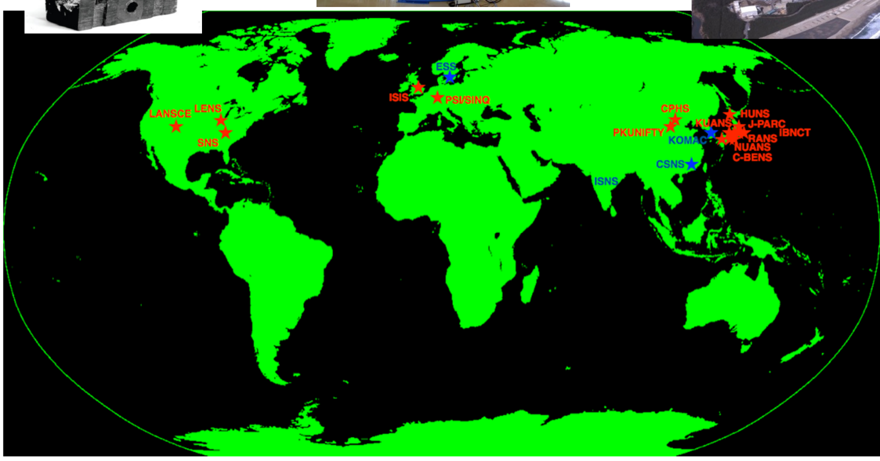
Rotating W target (not liquid Hg).

Same average intensity as high-power research reactor (ILL, HFIR).

~30x in peak intensity.

Parallel Developments: Compact Sources

Unlike synchrotrons, neutron sources still do not have a small-scale laboratory equivalent



From http://ucans.org

Note proliferation of smaller sources in Far East.

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RANS: RIKEN Accelerator Neutron Source

Be target: direct nuclear reaction (not spallation per se).

Very compact: 15 m long, 2 m wide (size of a neutron instrument at a large facility)

Sufficient flux for a number of applications in non-destructive testing of materials, neutronics R&D.

http://rans.riken.jp/en/rans.html

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Recap of Lecture I

- Thermal neutrons are an exquisite probe of condensed matter (more next lecture).

- Neutrons are hard to produce → no lab-based source (yet), need dedicated facilities at central laboratories.

- Accelerator-based neutron (and muon) sources offer higher fluxes of (useful) neutrons

- Golden Age for accelerator-driven neutron (and muon) sources, both large-scale and compact.

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Next Lecture

- Condensed matter research with neutrons: why, what, and how.
- Neutron production: challenges and opportunities.
- Recap: what you should remember a year from now

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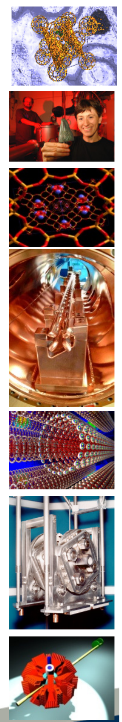

Accelerator-based Neutron Sources for Condensed Matter Research

Lecture II: Neutrons for Science

Felix Fernandez-Alonso

ISIS Pulsed Neutron & Muon Source
Rutherford Appleton Laboratory
Science and Technology Facilities Council

Applications of Accelerators
Cockcroft Institute Lecture Series
Winter Term 2015

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Outline – Lecture II

- Condensed matter research with neutrons: why, what, and how.
- Neutron production: challenges and opportunities.
- Recap: what you should remember a year from now.

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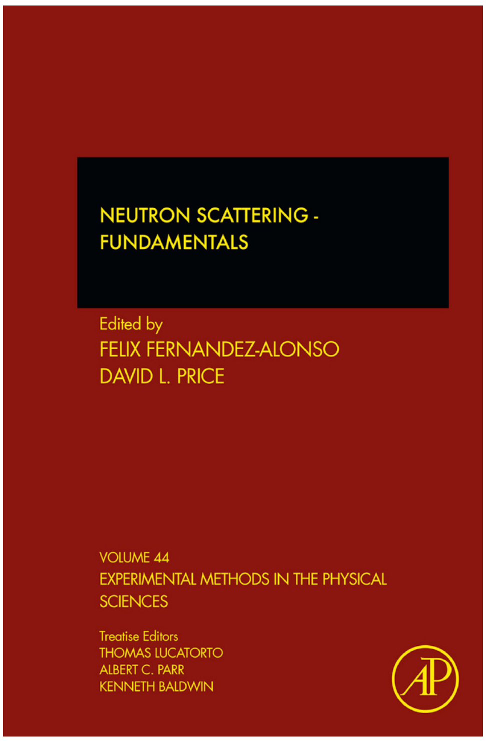
For Much More




Contents

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Condensed Matter Science at a Spallation Neutron Source

ISIS Experimental Halls

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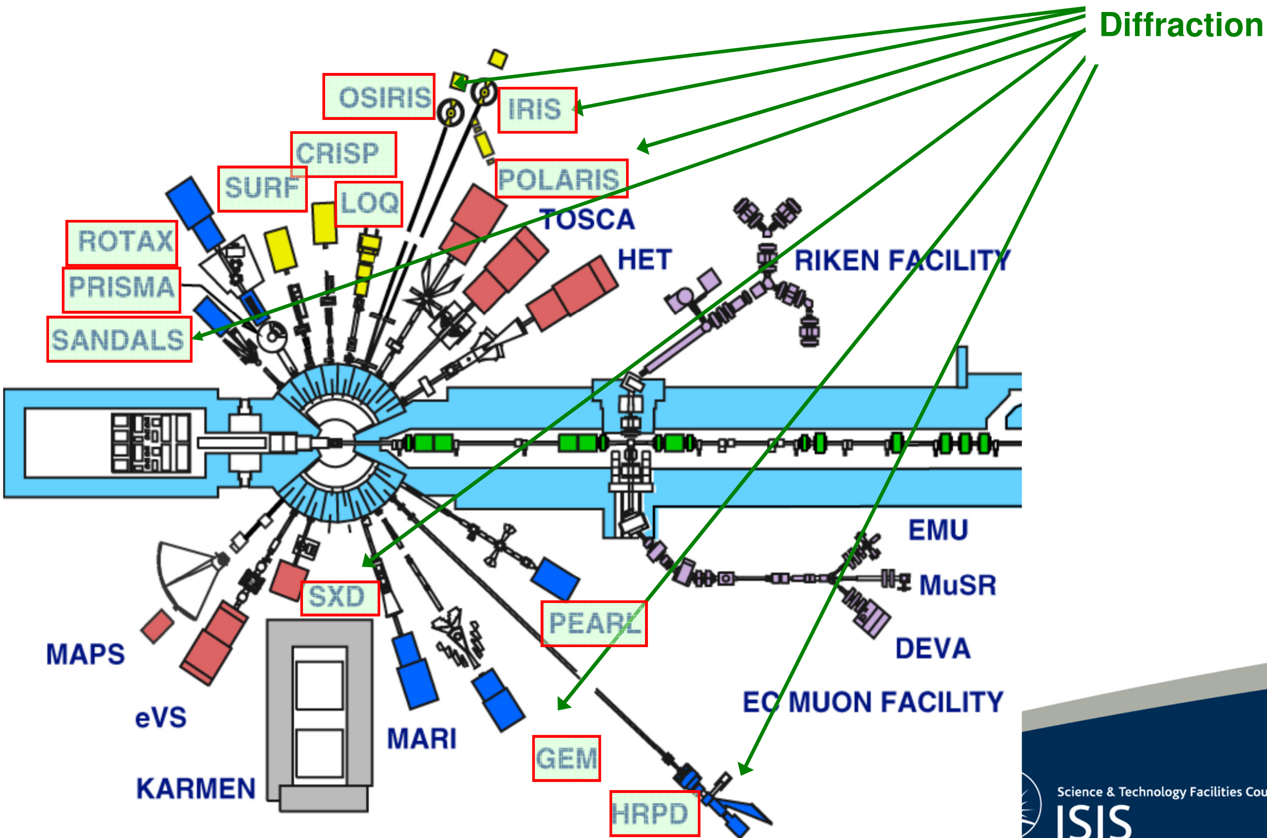
ISIS Neutron Instruments: Where Atoms Are (Structure)



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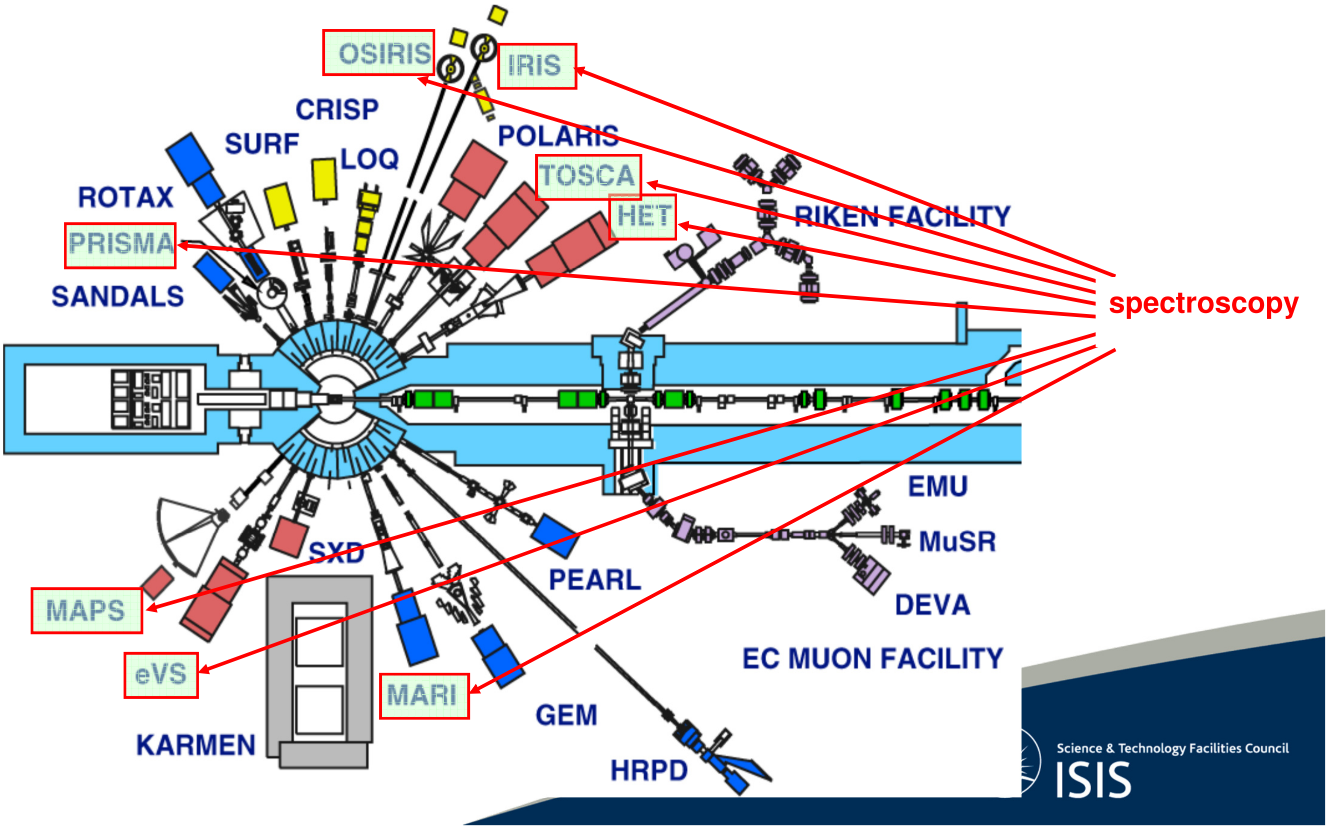
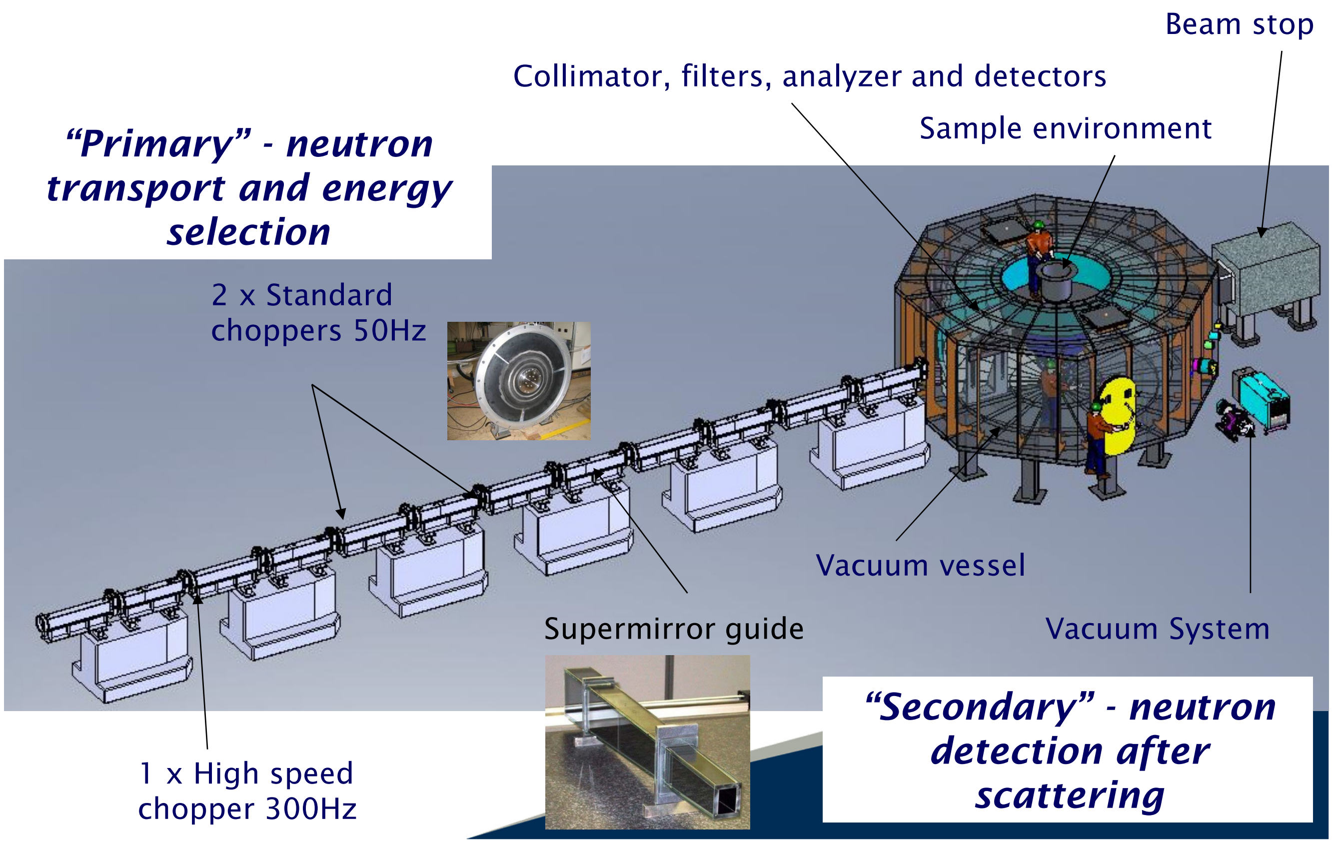
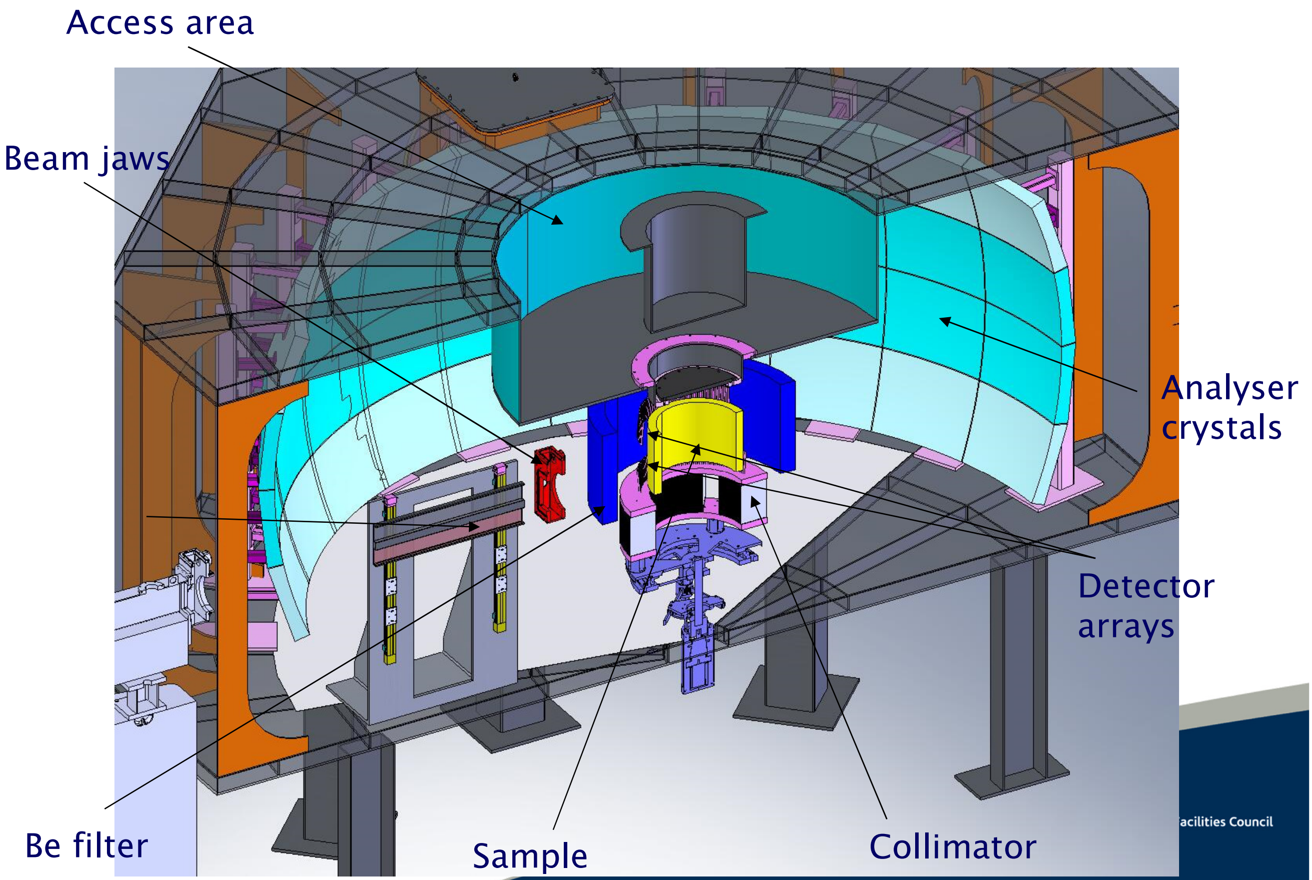
ISIS Neutron Instruments: What Atoms Do (Dynamics)



Back to Neutrons: The Anatomy of an Instrument

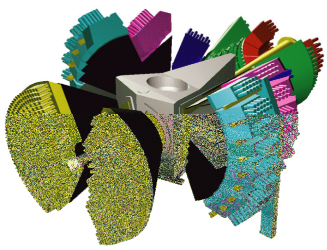


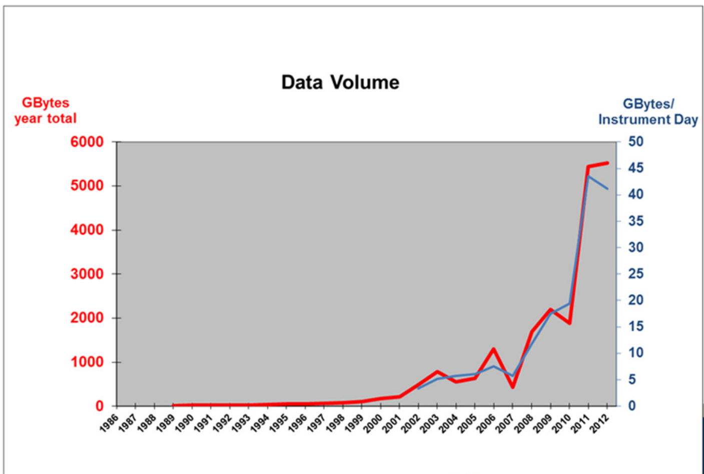
The Anatomy of a Neutron Instrument: The "Secondary"

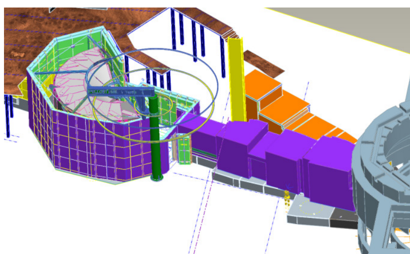


The "Tertiary" Instrument: Data Mining & Analysis

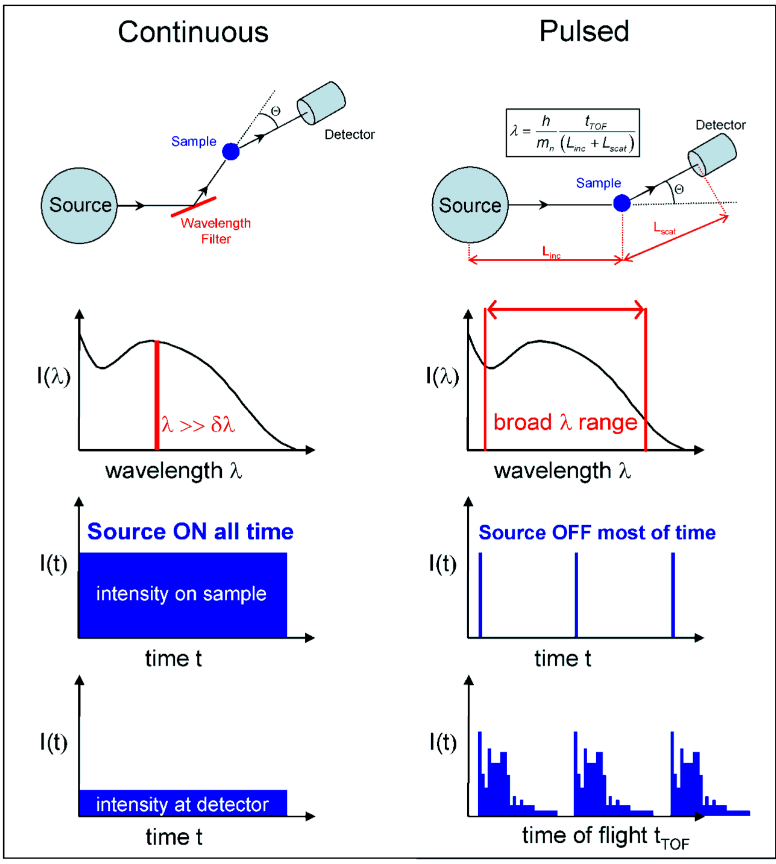
- Multi-dimensional data sets (5d and above!).
- New data collection paradigms, e.g., event mode.
- Extensive use of distributed computing & computer modelling.







The Merits of Pulsed Neutrons



Pulsed Sources:

- Time-of-flight spectrum is trivially related to neutron wavelength spectrum.
- Broad range of neutron energies (from meV to eV).
- Tight pulses: good resolution.
- Multiplexing advantage: broad range of wavelengths can be used simultaneously (more efficient experiments)
- Source is OFF most of the time (backgrounds are low).
- Source repetition frequency determines dynamic range.

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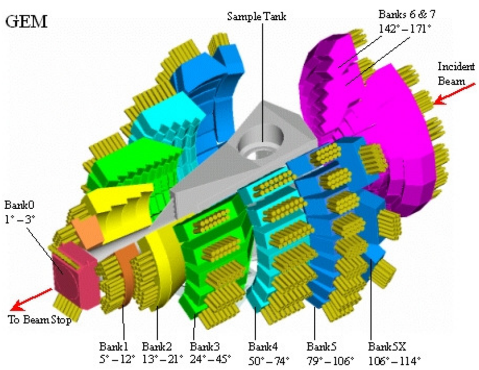
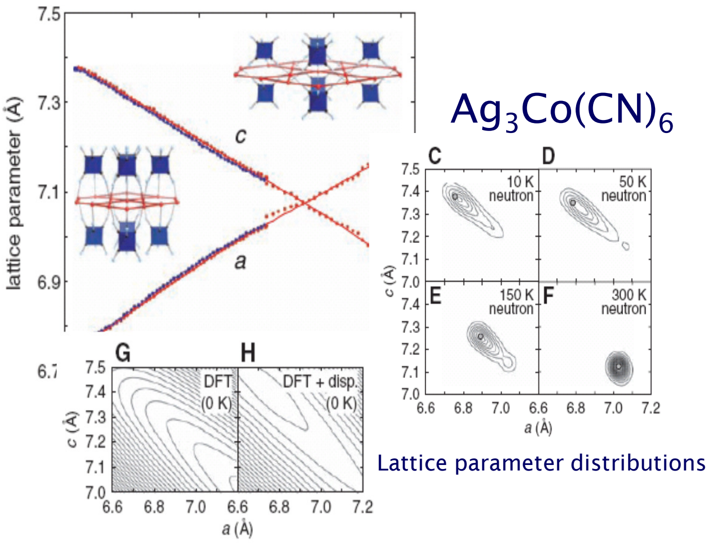
The Advantages of Multiplexing: Diffraction

- Large solid angle coverage
- High count rate
- Extended Q-range



- Liquid methane moderator.
- Primary flight path L_1=17.0 m
- Detectors group in 7 banks from 2q=1.1 to 169 degrees.
- ~7290 detectors
- Solid angle 1.1π steradians

Colossal Thermal Expansion in Framework Materials



Lattice parameter distributions

Science **319**, 794 (2008).

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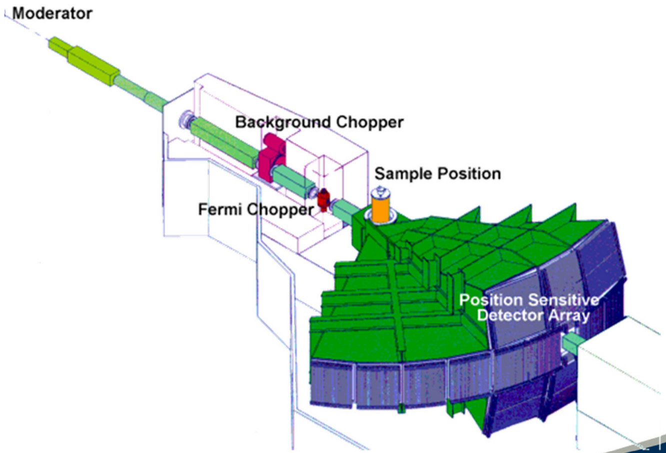
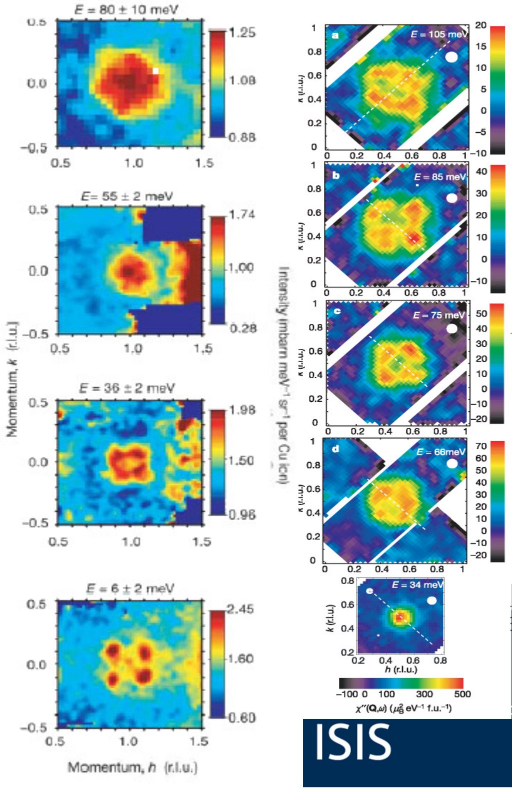
The Advantages of Multiplexing: Spectroscopy

- Excitations in single crystals
- Wide energy range 20meV – 2eV
- Low backgrounds
- Large solid angle of detectors
  - Low angle banks 3° – 30°
  - High angle banks 30° - 60°
- 40,000 pixelated detectors, 100 million points per dataset.



High-T_c Superconductivity (Cuprates)

$La_{2-x}Ba_xCuO_4$ $YBa_2Cu_3O_{6+x}$



Quantifying Success

$$S \propto \prod_i F_i$$

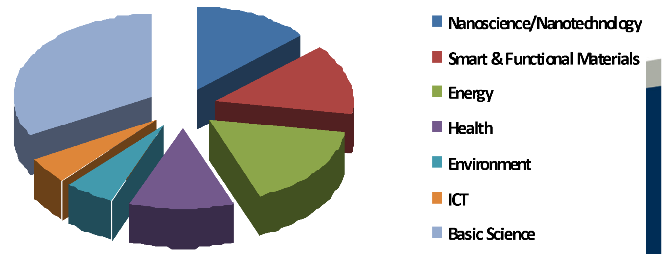
where the factors F_i include:

- Source power (e.g., kW vs MW)
- Reliability (machine downtime, harder than in a reactor)
- Optimisation (e.g., neutron moderation & transport)
- Instrumentation
- Planning
- Innovation
- Investment
- Scientific leadership
- User community
- Support facilities
- Staff expertise
- Cost effectiveness

The Impact of Neutron Science

Global challenges	ISIS
Energy	13% ✓✓✓✓
Living with environmental change	5% ✓✓✓
Global threats to security	0.5% ✓
Ageing: Life-long health and wellbeing	6% ✓✓
Digital economy	9% ✓✓✓
Nanoscience: through engineering to application	8% ✓✓✓

As well as a good balance with fundamental & curiosity-driven research.



ISIS and Industry

Access for industrial customers

ISIS Collaborative R&D Programme
The main route of for industry to access ISIS is through the Collaborative R&D programme. It allows companies to explore how neutrons could help their research, capitalising on ISIS expertise in carrying out experiments and data analysis. ISIS scientists assist users through the experimental process, and also have an extensive network of contacts in academia. This helps companies wanting to form new collaborations to find people working in their field.

Guidelines for writing an ISIS Collaborative R&D proposal
Requests for ICR&D beam time can be made at any time and will be considered outside the normal ISIS academic peer review process.

Optimising machining strategies for Boeing
Friday 08 August 2014
Understanding the development and distribution of residual stresses caused by machining is key to improving machining processes. The Advanced Manufacturing Research Centre (AMRC), with Boeing, at the University of Sheffield have been using Engin-X at ISIS to study the evolution of residual stresses in AA7050 – an aluminium alloy commonly used in aerospace structures - as it is heated and then machined. This understanding will enable them to reduce non-conformance in the manufacturing process, and significantly reduce costs.

Breaking the Barriers to a solar Future
Wednesday 23 July 2014
Researchers at the University of Sheffield, University of Durham and ISIS in collaboration with Start-up Company Ossila are using neutron reflectometry to look the formation of plastic solar cell films with the goal of developing devices which efficiently harness the power of the sun whilst being cheaper and easier to manufacture than the current silicon solar cells.

The Linde Group launches revolutionary carbon nanotube ink with help from ISIS
The Linde Group, a world-leading gases and engineering company, has launched SEERe-Ink, a revolutionary ink based on carbon nanotubes for use in flat screen TVs, touchscreens and solar cells.

Helping make hydrogen cars a reality
Tuesday 04 February 2014
Toyota, who hope to release a hydrogen fuel cell vehicle in 2015, have been working with ISIS scientists to address a key challenge: hydrogen loss during cycling.

Building safer ships with Lloyd's Register
Tuesday 22 July 2014
Ultrasonic peening (UP) is a technique for improving the fatigue performance of welded joints. Little research has been done on how UP-treated welds behave when they are subjected to real world conditions such as compressive overload or variable amplitude loading. Lloyd's Register provides quality assurance to the marine industry, and they have been using ENGIN-X to investigate UP welded joints in these conditions. Understanding the process and its benefits will allow improved control of fatigue cracking, lower maintenance costs, and extending the life of welded connections in marine and other industries.

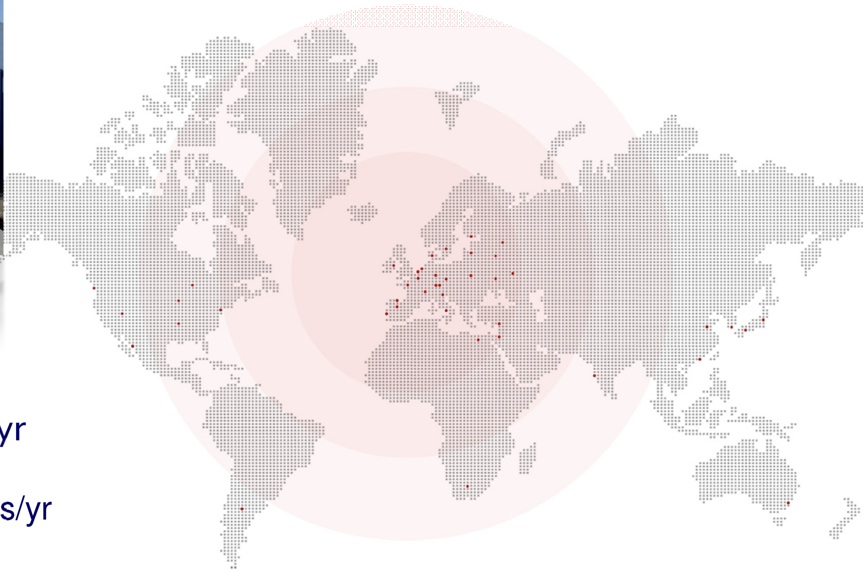
Solar flares, muons and micro-electronics – what's the connection?
Friday 17 May 2013
Here on Earth, such spectacular solar flares seem far away but in fact these extra-terrestrial events are a cause for concern in our modern digital world.

Testing new welding techniques for the nuclear industry with AREVA
Monday 21 July 2014
Introduction of new designs, novel fabrication methods or modifications to existing plant in the nuclear power generation industry are subject to intense scrutiny to ensure that safety is not compromised. Multi-national corporation AREVA has designed the new European Pressurised Reactor (EPR) to meet stringent demands for increased safety and reduced cost of electricity generation. A twin EPR power station at Hinkley Point in Somerset is planned and will be constructed using modern welding technology.

www.isis.stfc.ac.uk/industry

Science & Technology Facilities Council ISIS

Some Metrics for ISIS



~1200 users/yr

~700 experiments/yr

150 days running (50 industry)

~450 publications/yr (1/3 high impact)

12,000+ publications to date

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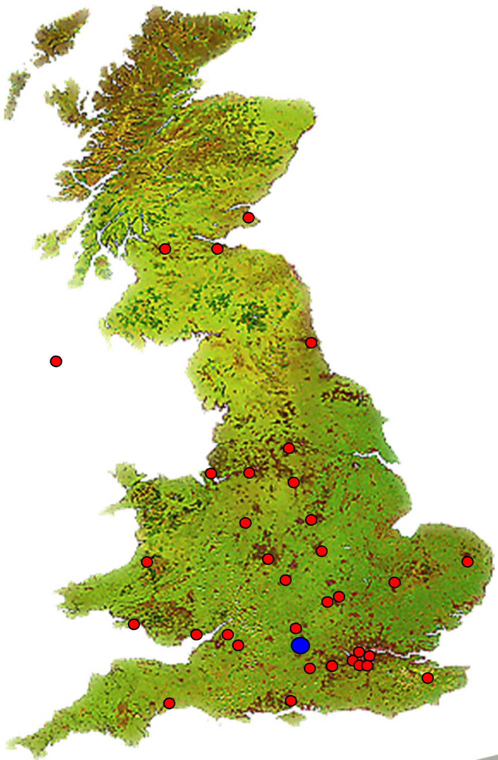
ISIS UK Community

Aberystwyth
Bath
Belfast
Birmingham
Bristol
Cambridge
Cardiff
Cranfield
Durham
East Anglia
Edinburgh
Exeter
Glasgow
Keele
Kent



Leeds
Leicester
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Nottingham
OU
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Reading
Sheffield
Southampton
St. Andrews
Surrey
Swansea
Warwick

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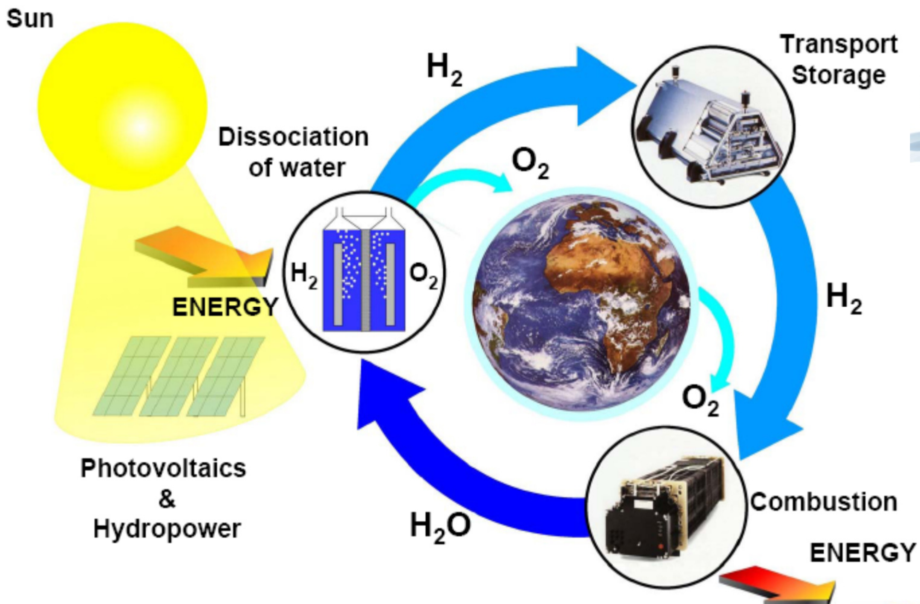
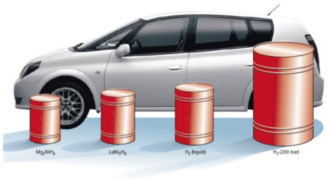
Global Challenges: The Hydrogen Dream

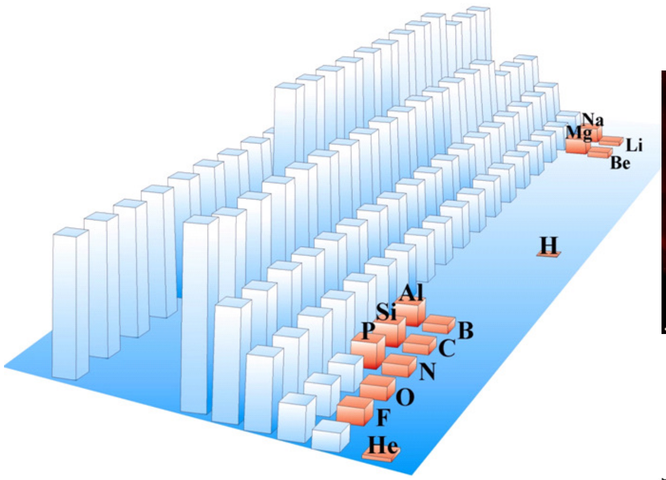




- Direct use of renewable energy sources (e.g., solar).
- Hydrogen as energy carrier or "vector."
- Combustion in fuel cell: efficient & green.
- Challenges: making, splitting, and storing hydrogen.

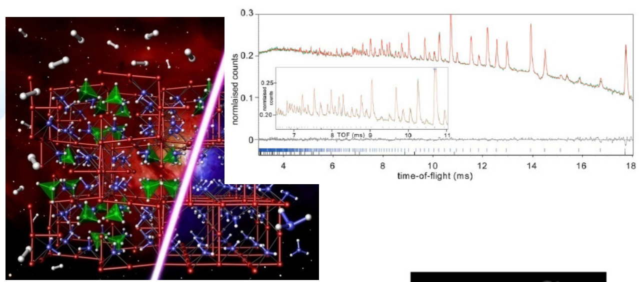
Energy Research: Hydrogen Storage

Light Elements
Need to locate H



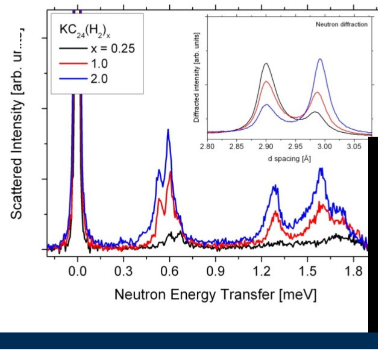
Structure of $Li_4BN_3H_{10}$ and $LiNH_2$

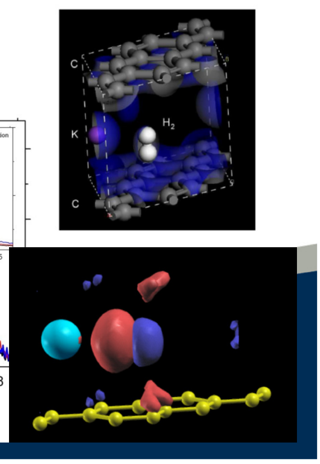
Chem Comm 2439 (2006)



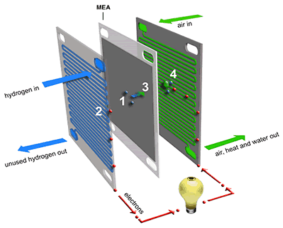
Binding sites of molecular hydrogen in metal-doped graphites from neutron spectroscopy

Phys Rev Lett 26101 (2008)



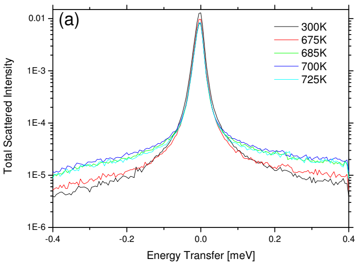


Energy Research: Fuel Cells & Battery Materials

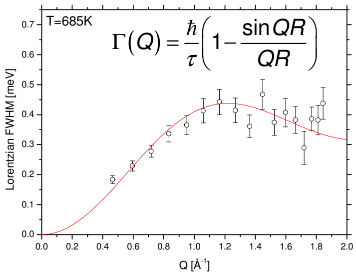


$LaSrCoO_3H_{0.7}$: transition metal oxide with a high H concentration.

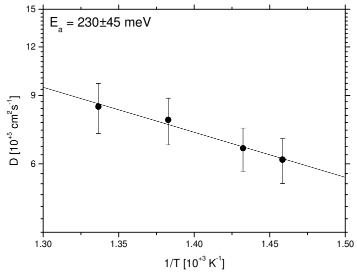
Neutron Spectra

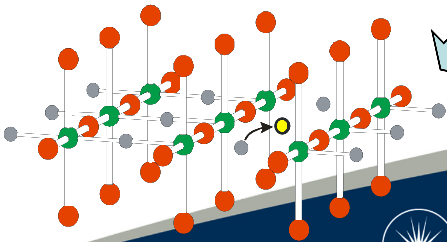


Hydride Diffusion



Energetics of Diffusion





Hopping mechanism

***Order-of-magnitude* increase in conductivity compared to other proton conductors.**

Advanced Materials 18 3304 (2006).

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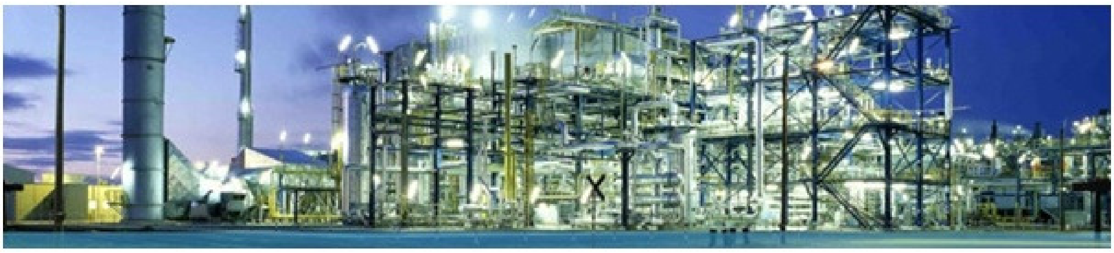
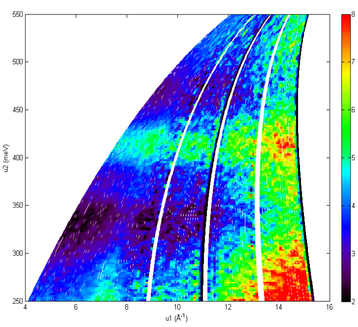
Dry Reforming of Methane

Hydrogen for the Hydrogen Economy

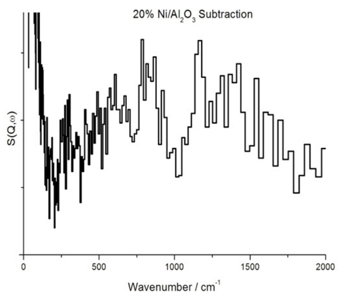


$CH_4 + CO_2$ → ($Ni(45\%)/Al_2O_3$) → CH_x → $CO + H_2$



Quantify hydroxyls and adsorbed hydrocarbon (MAPS)

Amorphous polymeric carbon (TOSCA)



David Lennon (Glasgow) et al.

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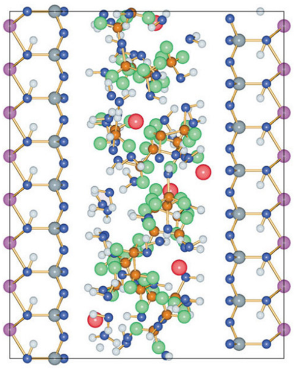
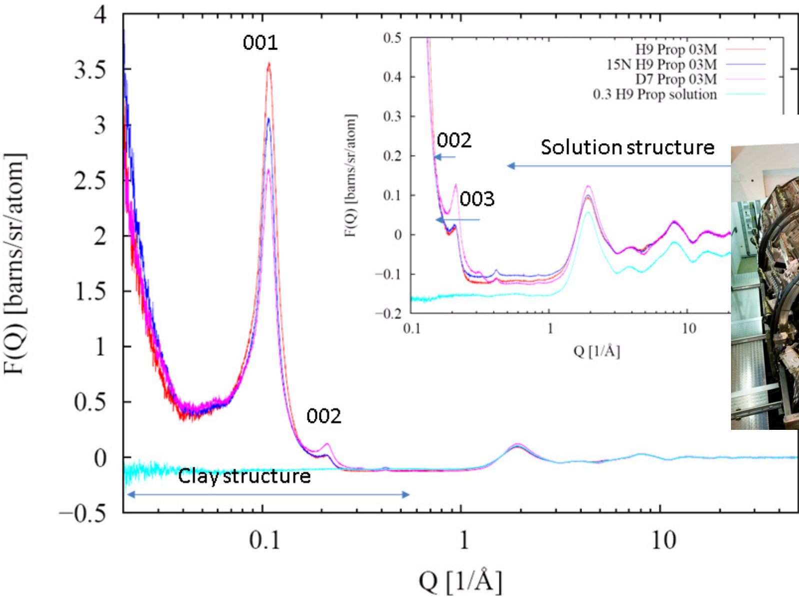
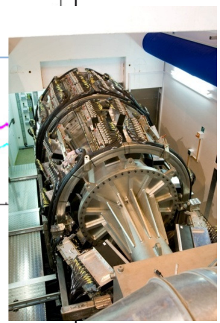
Environmental & Earth Science

Swelling Clays







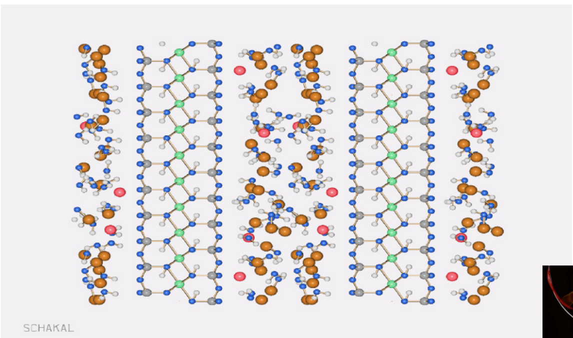
Atomistic models require knowledge of short and long length scales.

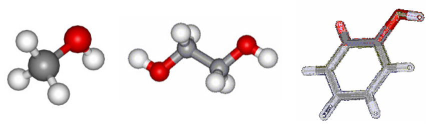
Applications to sequestration & waste remediation

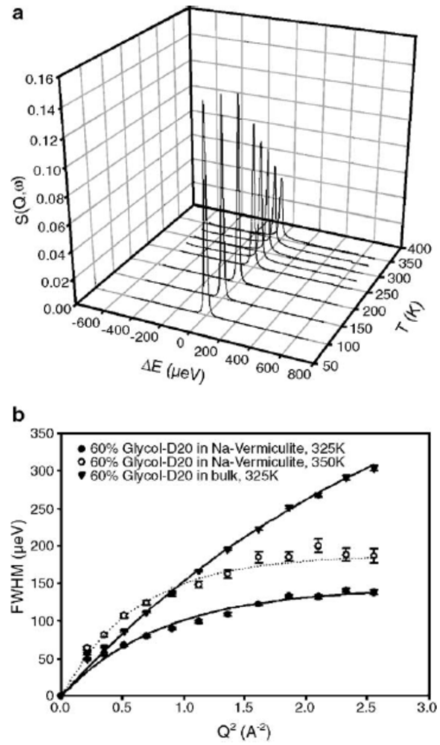
Only at a pulsed neutron source.

Science & Technology Facilities Council ISIS

Neutrons and Soil Pollution







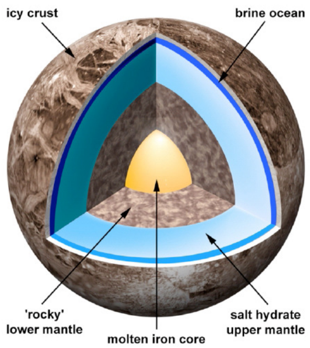
- Diffusion of organic molecules (hydrogenous): unique to neutron spectroscopy.
- Ability to emulate geophysical environments below Earth's crust.

Science & Technology Facilities Council ISIS

NT Skipper, PA Lock, et al, *Chemical Geology* **230** (2006) 182.

Extreme Conditions, on Earth and Beyond

Modelling Planetary Interiors



The largest icy moons

(radii ~ 2500 km);

Ganymede

Callisto

Titan

'Ice' mantles

~ 800 - 900 km deep

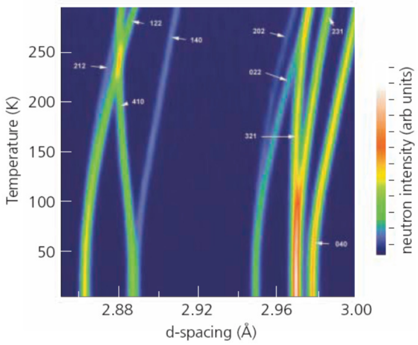
Core mantle P

~ 1.5 – 2.0 GPa

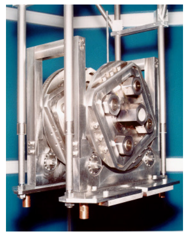
Core mantle T

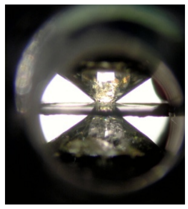
~ 300 K

Epsom Salt ($MgSO_4$ $7H_2O$) and the Moons of Jupiter

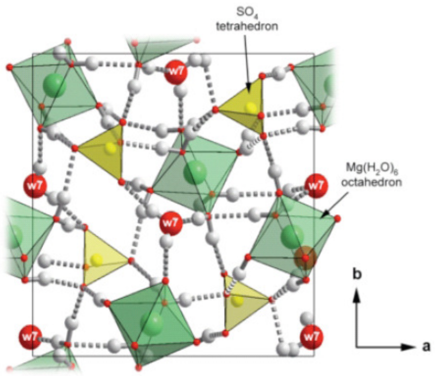


High-pressure Cells

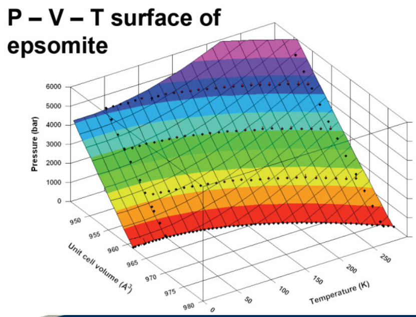




Structure



Phase Diagram



Facilitated by penetrating power neutrons.

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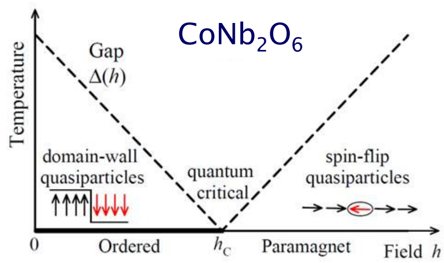
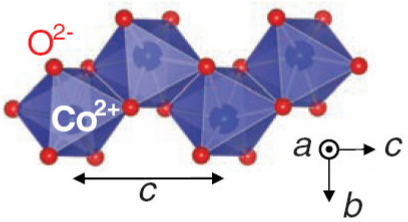
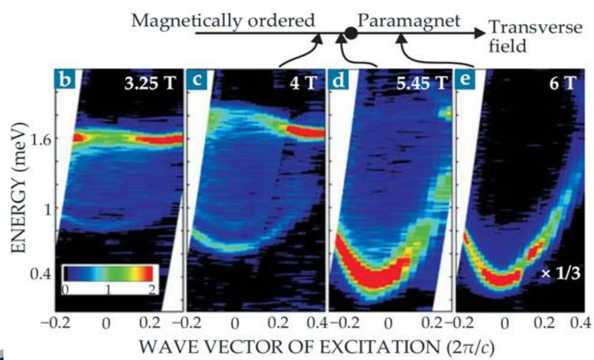
Extreme Conditions: Quantum Matter

Strongly Correlated Systems & Quantum Phase Transitions



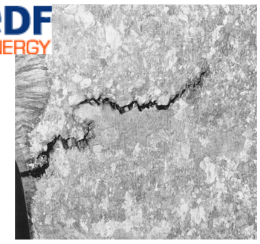
High B-fields and low Ts required

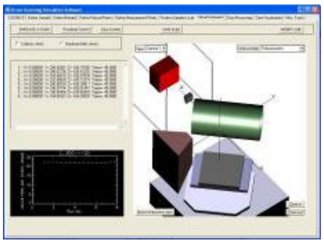
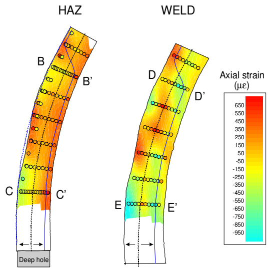


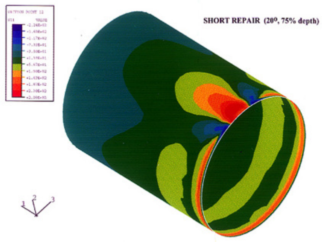


Engineering: Stress, Strain, and Materials Performance

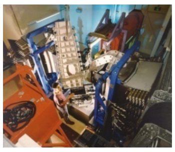
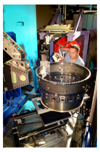
Diagnosing cracks in advanced gas-cooled reactors

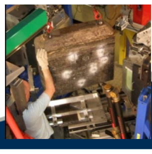




AIRBUS
Rolls-Royce
LUCCHINI RS GROUP
Magnesium Elektron



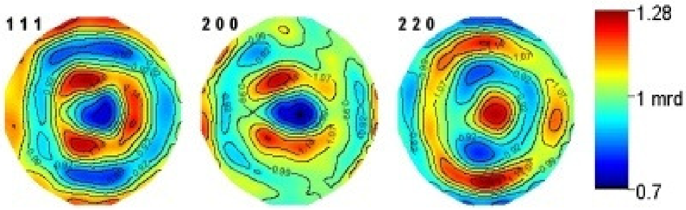
Courtesy of SY Zhang (ISIS)

Neutrons and Archaeology

Analysis of Ancient Greek Helmets


National Museum of Wales, Cardiff

Manchester Museum

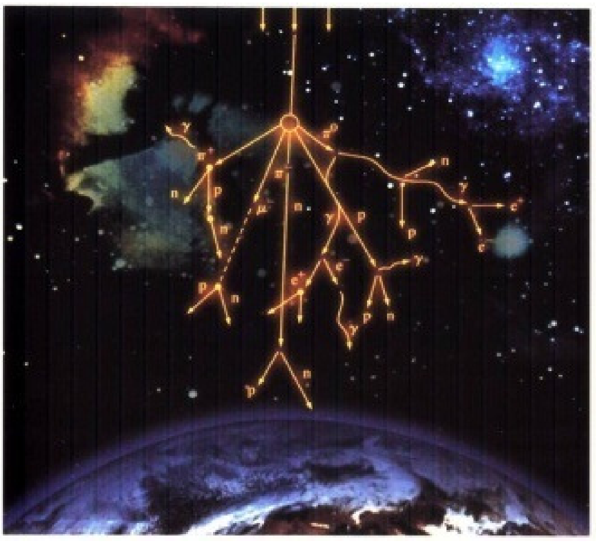


Texture of Archaic Greek helmet

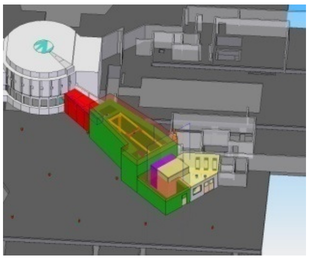
Questions :

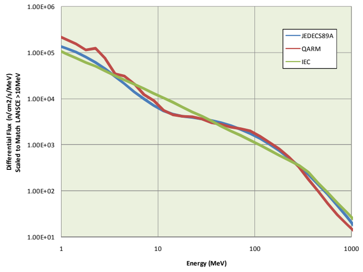
- Origin: Archaic or Classical period?
- Technology: single piece of bronze?
- Preservation state: harmful corrosion products?
- Authenticity: are these the original?

Neutrons Helping the Semiconductor Industry



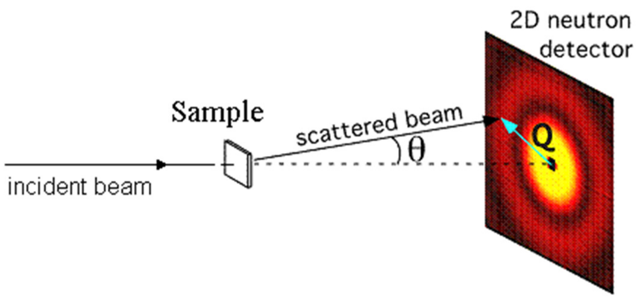
- Atmospheric neutrons collide with microchips and upset microelectronic devices every few seconds.
- 300x at high altitudes.
- Spallation sources provide same fast neutron spectrum at much higher intensities (1 ISIS-hr ~ 100 years.)
- Manufacturers can mitigate against the problem of cosmic radiation.

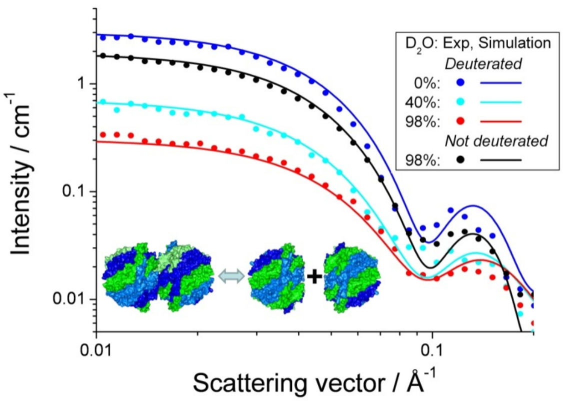




From Atoms to the Bulk: Small-angle scattering

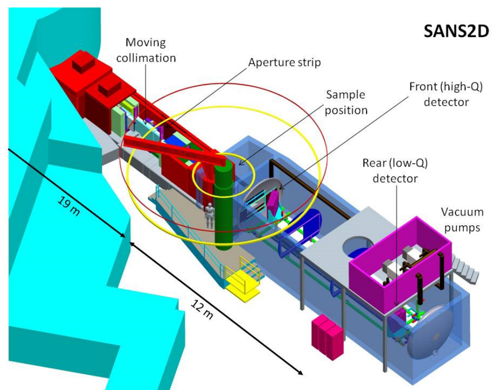
- Small-angles → low momentum transfers → large length scales *d*.
- Best done with cold neutrons as $d \sim \lambda/\theta$
- Ultra-small angles can be achieved by using the neutron spin to encode scattering angle.





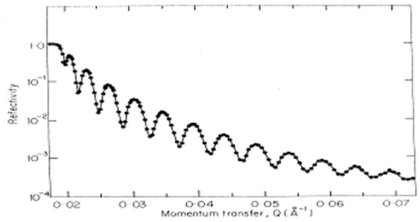
Solution structure of proteasome activators (Sugiyama et al.)

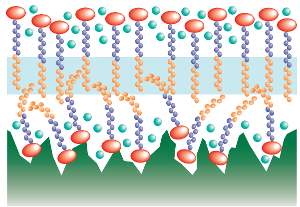
Vast and increasing number of applications biology and soft matter.

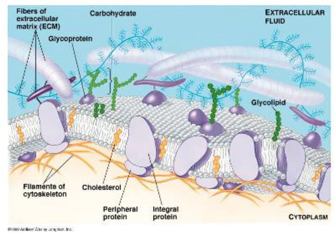


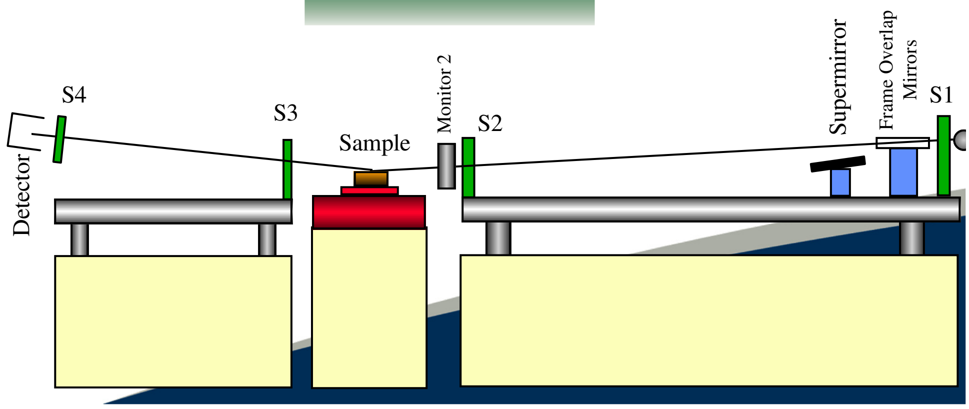
From Atoms to the Bulk: Reflectometry

- Same principle as in optical reflectivity, contrast is very different (e.g., H/D substitution).
- Ability to study buried interfaces.
- Ideal for studies on soft-matter: air-liquid and liquid-liquid interfaces in soaps, detergents, shampoos, biological membranes …



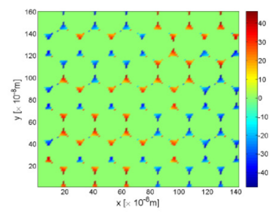


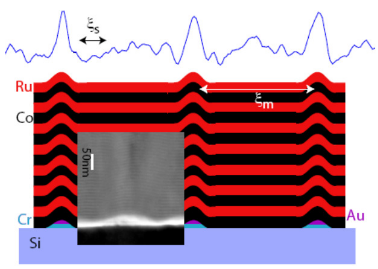




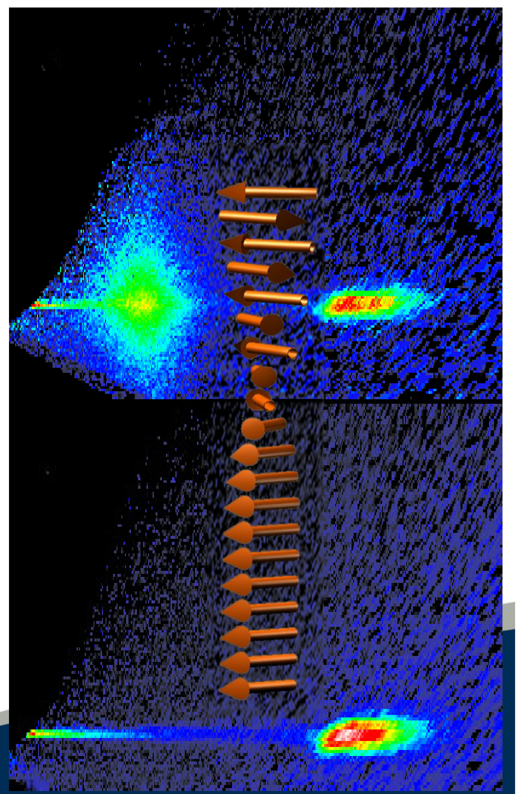
From Atoms to the Bulk: Magnetic Reflectometry

Magnetic Layered Materials

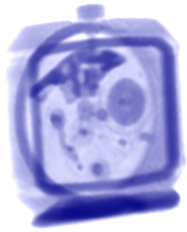




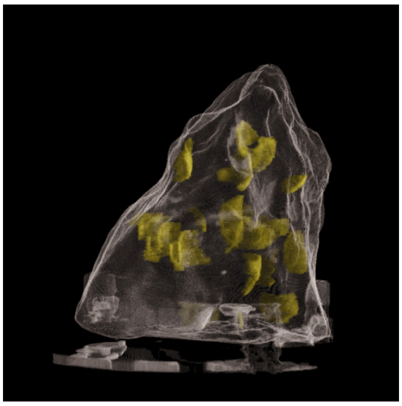
- Exploits sensitivity of neutron to unpaired spin density (via polarisation analysis).
- Probes length scales from nm to μm: domain structure, interfacial magnetism, spin transport, proximity effects, …

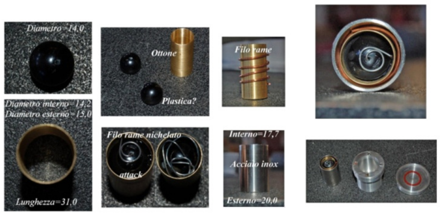


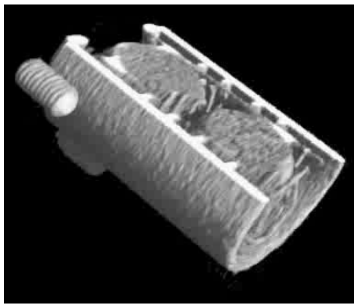
Well into the Bulk:
Neutron Imaging and Tomography

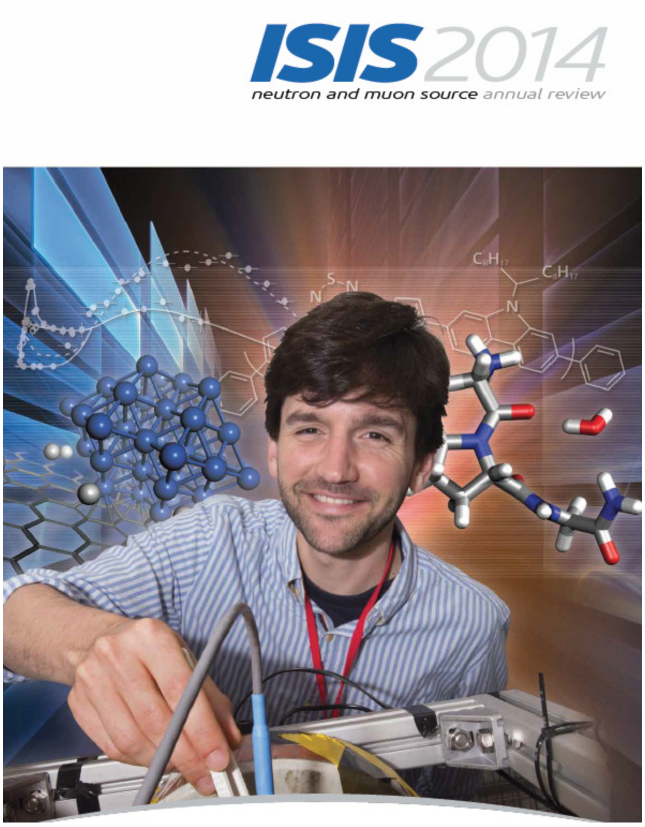


- Imaging and diffraction techniques.
- Materials science, engineering, geology and archaeological sciences.
- Energy resolved imaging.
- Separate materials and phases.









www.isis.stfc.ac.uk

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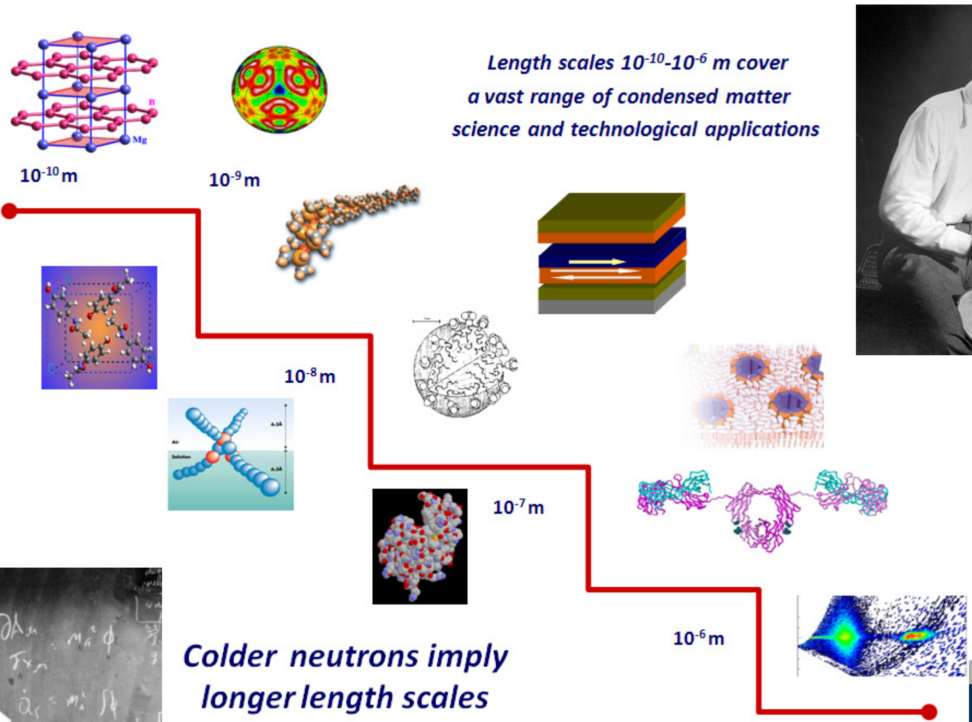
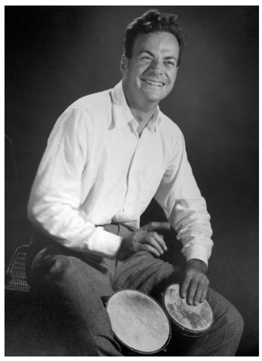
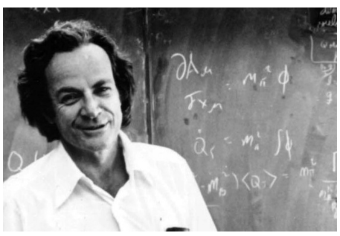
Challenges & Opportunities

There is Plenty of Room at the Bottom – *RP Feynman*

Length scales 10^{-10}-10^{-6} m cover a vast range of condensed matter science and technological applications







Colder neutrons imply longer length scales

The Evolutionary Way

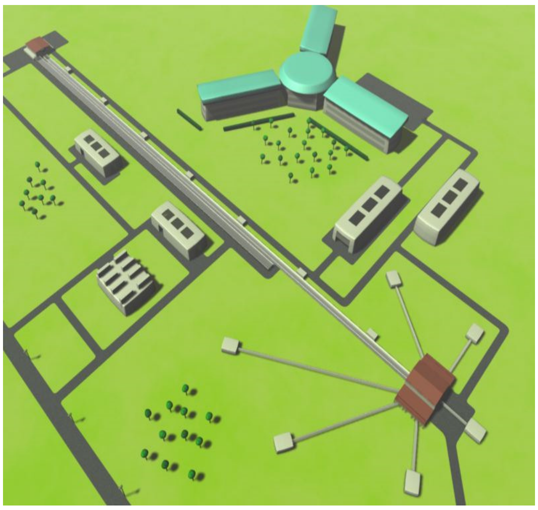
ISIS (UK): hot (1984) & cold (2008)

PSI (Switzerland): warm, cold & ultracold

LENS (USA): cold/ultracold

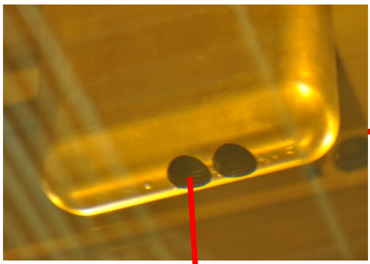
SNS (US): hot (2007) & cold (under consideration)

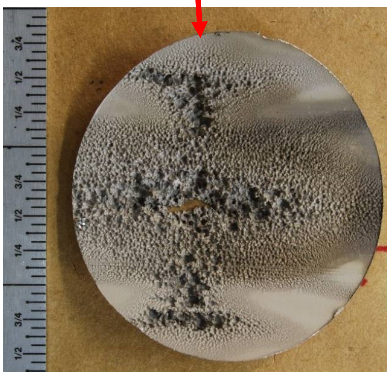
Beyond Evolution: ESS

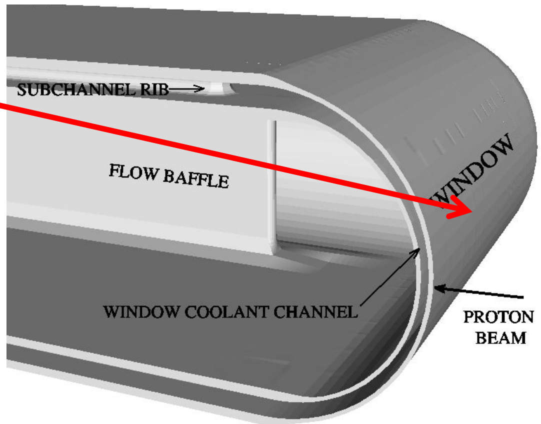


- Intense spallation source optimised for cold neutrons.
- Specification: 5 MW, 2.8 msec pulses (H Linac).
- Target station with up to 40 instruments (typical length 200 m).
- Complementary to short-pulse sources (JPARC, SNS, ISIS).
- Large investment, in construction phase (Lund Sweden).
- Challenges:
  - Power dissipation at 5MW: latest solution is a rotating tungsten target.
  - Instrument concepts largely untested to fully exploit 'long pulse.'

Liquid Mercury Targets and the Challenge of MW Sources

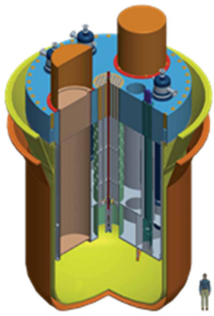






Ramping up power above 1 MW has been a challenge, requiring extensive R&D (He bubbling to avoid cavitation, etc)

Emerging (Hybrid) Concepts



http://myrrha.sckcen.be/

Construction envisaged 2017-2021

Full operations 2025

960 M€

Fast-neutron reactor 50-100 MW$_{th}$.

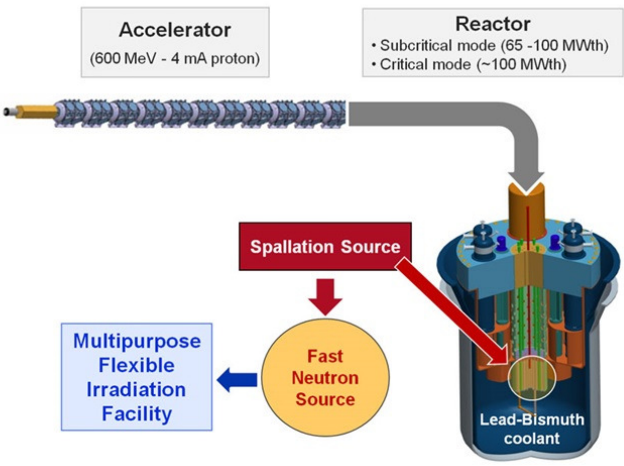
600 MeV, 4 mA ADS (SC proton LINAC)

Spallation target + multiplying MOX core.

Transmutation & radioactive waste.

Replaces BR2 isotope reactor.

Plans for a similar facility by JAEA (Japan)



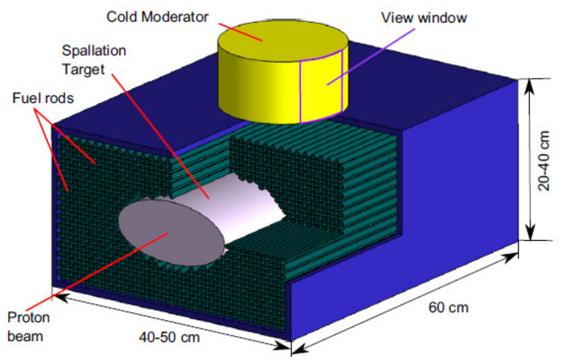
ADS-based Neutron Facilities

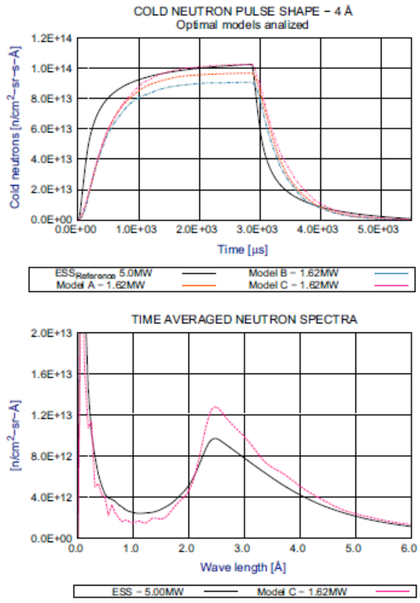
Nuclear Instruments and Methods in Physics Research A 767 (2014) 176–187

Basic concept for an accelerator-driven subcritical system to be used as a long-pulse neutron source for Condensed Matter research

R. Vivanco [a,b,*], A. Ghiglino [a,b], J.P. de Vicente [a,b], F. Sordo [a,b], S. Terrón [a,b], M. Magán [a,b], J.M. Perlado [b], F.J. Bermejo [c]

[a] ESS-BILBAO, Parque Tecnológico Bizkaia, Laida Bidea, Edificio 207 B Planta Baja, 48160 Derio, Spain
[b] Instituto de Fusión Nuclear - UPM, ETS Ingenieros Industriales, C/ José Gutiérrez Abascal, 2, 28006 Madrid Spain
[c] Instituto de Estructura de la Materia, IEM-CSIC, Consejo Superior de Investigaciones Científicas, Serrano 123, 28006 Madrid, Spain





Cost effective solution.

Use of fissile fuel (regulatory implications)

Neutron pulse shape metrics for different ADS configurations. Neutrons between 4 Å on cold moderator surface.

	ESS	Model A	Model B	Model C
Peak (n/cm²/Å/sr/s)	10.30×10^{13}	9.68×10^{13}	9.10×10^{13}	10.30×10^{13}
Signal (n/cm²/Å/sr)	2.54×10^{11}	2.26×10^{11}	2.13×10^{10}	2.37×10^{10}
Tail (n/cm²/Å/sr)	4.25×10^{10}	5.74×10^{10}	4.86×10^{9}	5.99×10^{9}
Signal to tail ratio	5.99	4.25	4.39	3.95
To 50% decrease (μs)	173	393	373	413
To 10% decrease (μs)	1003	1073	1063	1163

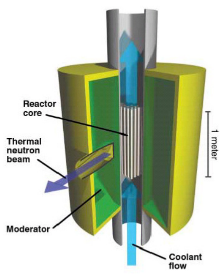
Beyond Spallation

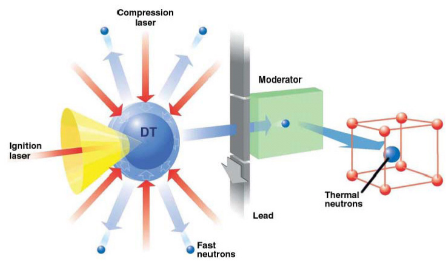
23 FEBRUARY 2007 VOL 315 SCIENCE

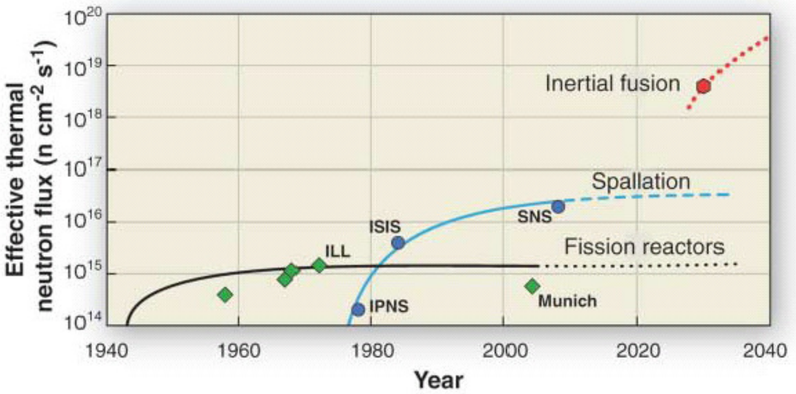
A Route to the Brightest Possible Neutron Source?

Andrew Taylor,[1*] Mike Dunne,[1] Steve Bennington,[1] Stuart Ansell,[1] Ian Gardner,[1] Peter Norreys,[1] Tim Broome,[1] David Findlay,[1] Richard Nelmes[2]

We review the potential to develop sources for neutron scattering science and propose that a merger with the rapidly developing field of inertial fusion energy could provide a major step-change in performance. In stark contrast to developments in synchrotron and laser science, the past 40 years have seen only a factor of 10 increase in neutron source brightness. With the advent of thermonuclear ignition in the laboratory, coupled to innovative approaches in how this may be achieved, we calculate that a neutron source three orders of magnitude more powerful than any existing facility can be envisaged on a 20- to 30-year time scale. Such a leap in source power would transform neutron scattering science.







Quantum leap in neutron production.

Implementation dependent upon further developments in fusion technology.

Science & Technology Facilities Council ISIS

For Much More

Major Neutron Sources for Condensed Matter Research

Accelerator-based

- Spallation Neutron Source (USA): neutrons.ornl.gov/facilities/SNS/
- ISIS Pulsed Neutron and Muon Source (UK): www.isis.rl.ac.uk
- Japan Spallation Neutron Source (Japan): j-parc.jp/MatLife/en/index.html
- Swiss Spallation Neutron Source (Switzerland): www.psi.ch/sinq/
- Los Alamos Neutron Science Centre (USA): lansce.lanl.gov/
- Low Energy Neutron Source (USA): www.indiana.edu/~lens/
- European Spallation Source (Sweden): ess-scandinavia.eu/
- European Spallation Source (Spain): www.essbilbao.com
- China Spallation Neutron Source (China): csns.ihep.ac.cn/english/index.htm

Reactor-based

- Institut Laue-Langevin (France): www.ill.eu/
- NIST Centre for Neutron Research (USA): www.ncnr.nist.gov/
- FRM-II (Germany): www.frm2.tum.de/en/index.html
- Bragg Institute (Australia): www.ansto.gov.au/research/
- High-flux Isotope Reaction (USA): neutrons.ornl.gov/facilities/HFIR/
- Laboratoire Léon Brillouin (France): www-llb.cea.fr/en/
- Berlin Neutron Scattering Centre (Germany): www.helmholtz-berlin.de

What You Should Remember a Year from Now

- Thermal neutrons are an exquisite probe of condensed matter.

- Neutrons are hard to produce → need dedicated facilities.

- Accelerator-based neutron sources:
    - Can also produce muons, also a unique probe of condensed matter.
    - Offer higher neutron flux → factors of ~10 justify new facilities.
    - Golden Age for neutron spallation, including compact sources.

- The success of an accelerator-based neutron source depends on many factors, not just source power.

- Spallation neutron sources like ISIS are science driven
    - Many science areas depend quite heavily on neutrons: hydrogen & magnetism.
    - New frontiers: bridging the gap between atoms and the bulk (the 'nano' domain).
    - To achieve this, we need more neutrons.

THE FUTURE LOOKS BRIGHT!

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Acknowledgements

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Questions, while we watch

Come & visit!

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