UT-BATTELLE

Fundamentals of Neutron Scattering Research

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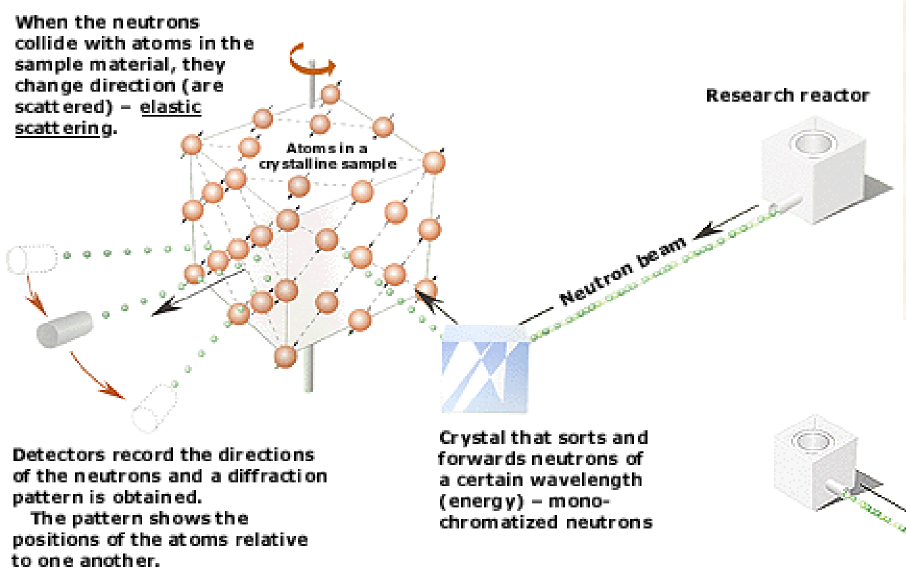
OAK RIDGE NATIONAL LABORATORY
U. S. DEPARTMENT OF ENERGY

What do neutrons do?

Nobel Prize in Physics 1994 - Shull and Brockhouse

Neutrons show where atoms are…..

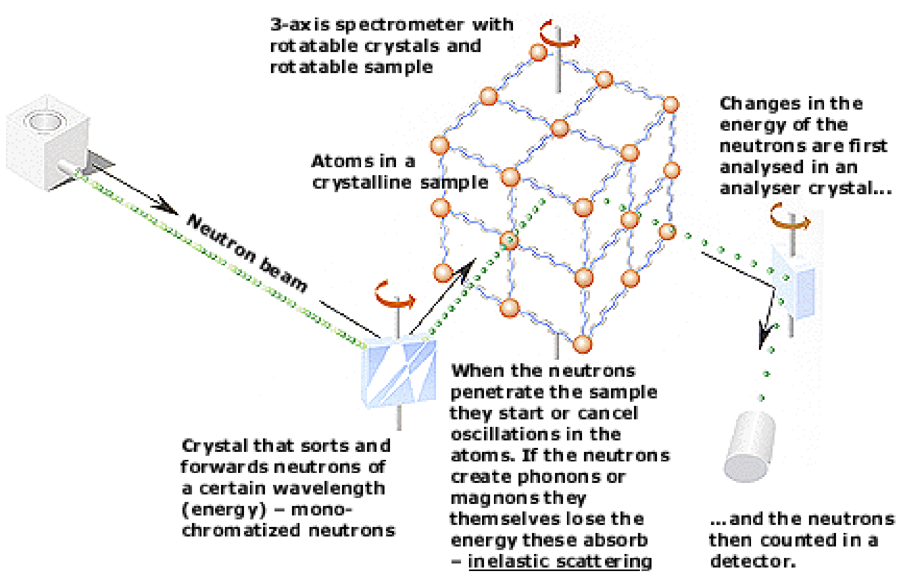


When the neutrons collide with atoms in the sample material, they change direction (are scattered) – elastic scattering.

Detectors record the directions of the neutrons and a diffraction pattern is obtained.
The pattern shows the positions of the atoms relative to one another.

Crystal that sorts and forwards neutrons of a certain wavelength (energy) – monochromatized neutrons

… and what atoms do



3-axis spectrometer with rotatable crystals and rotatable sample

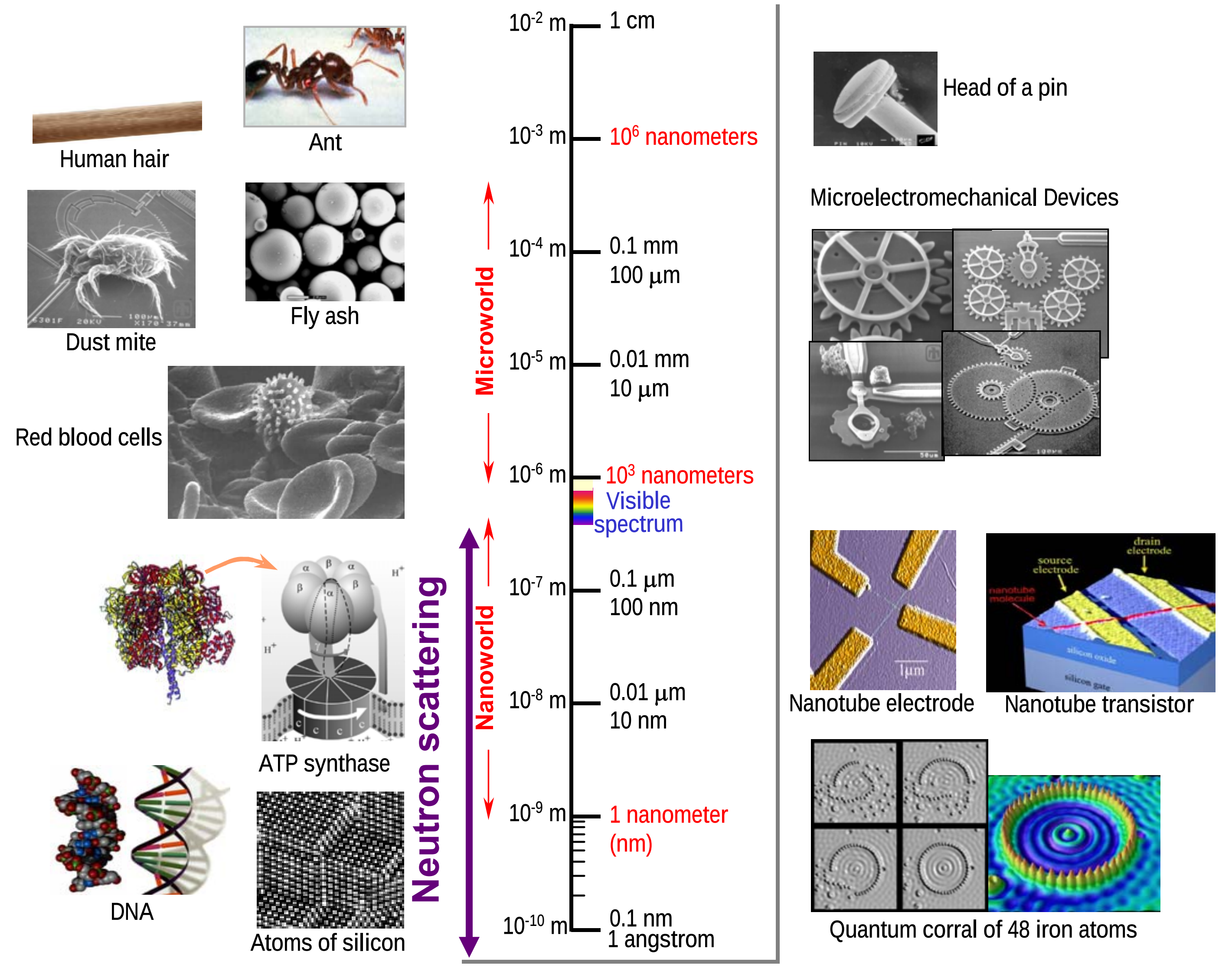
Changes in the energy of the neutrons are first analysed in an analyser crystal...

Crystal that sorts and forwards neutrons of a certain wavelength (energy) – monochromatized neutrons

When the neutrons penetrate the sample they start or cancel oscillations in the atoms. If the neutrons create phonons or magnons they themselves lose the energy these absorb – inelastic scattering

...and the neutrons then counted in a detector.

Neutrons: microns to angstroms!



10^{-2} m — 1 cm

10^{-3} m — 10^6 nanometers

10^{-4} m — 0.1 mm, 100 µm

10^{-5} m — 0.01 mm, 10 µm

10^{-6} m — 10^3 nanometers

Visible spectrum

10^{-7} m — 0.1 µm, 100 nm

10^{-8} m — 0.01 µm, 10 nm

10^{-9} m — 1 nanometer (nm)

10^{-10} m — 0.1 nm, 1 angstrom

Microworld

Nanoworld

Neutron scattering

Human hair

Ant

Dust mite

Fly ash

Red blood cells

ATP synthase

DNA

Atoms of silicon

Head of a pin

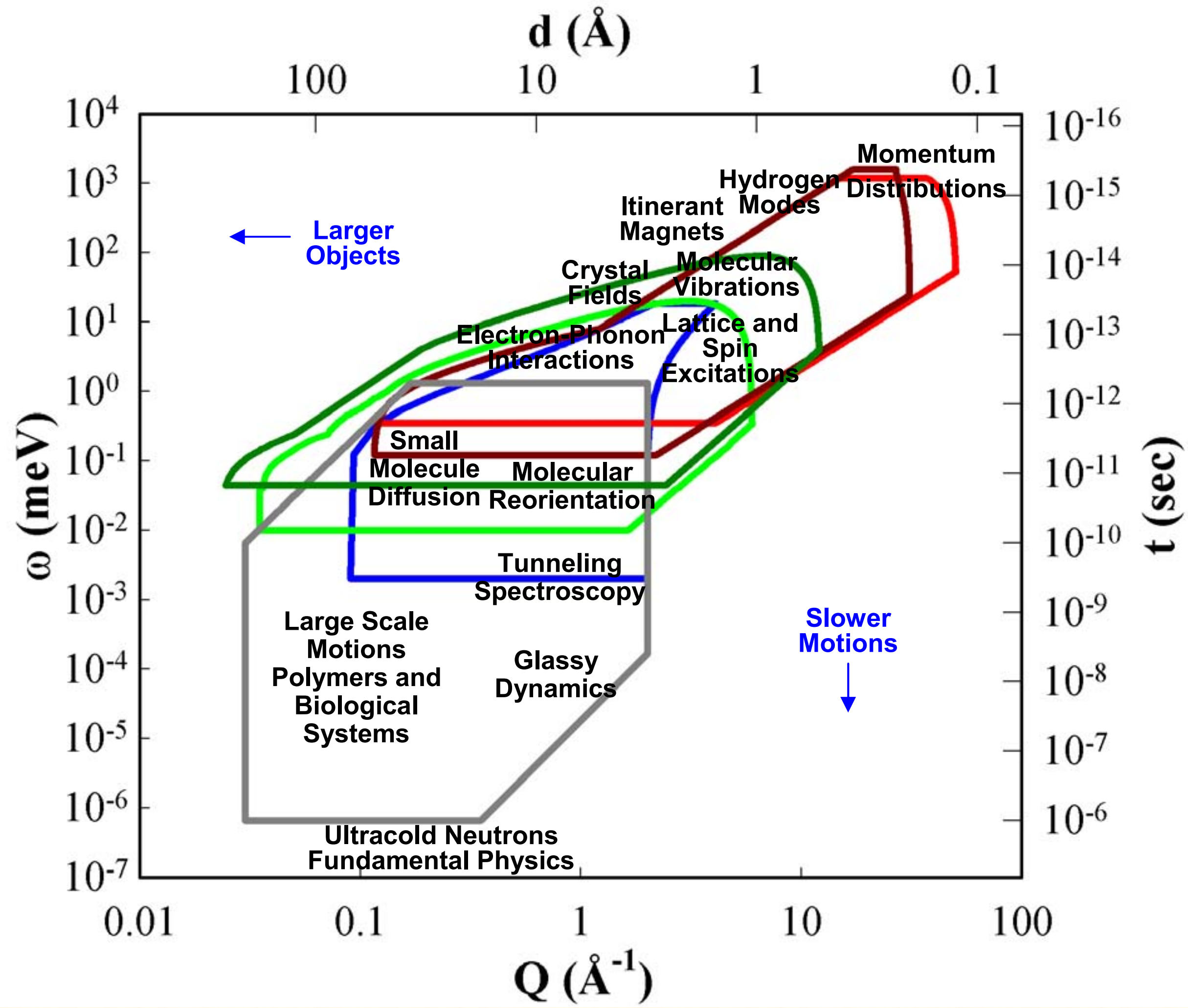
Microelectromechanical Devices

Nanotube electrode

Nanotube transistor

Quantum corral of 48 iron atoms

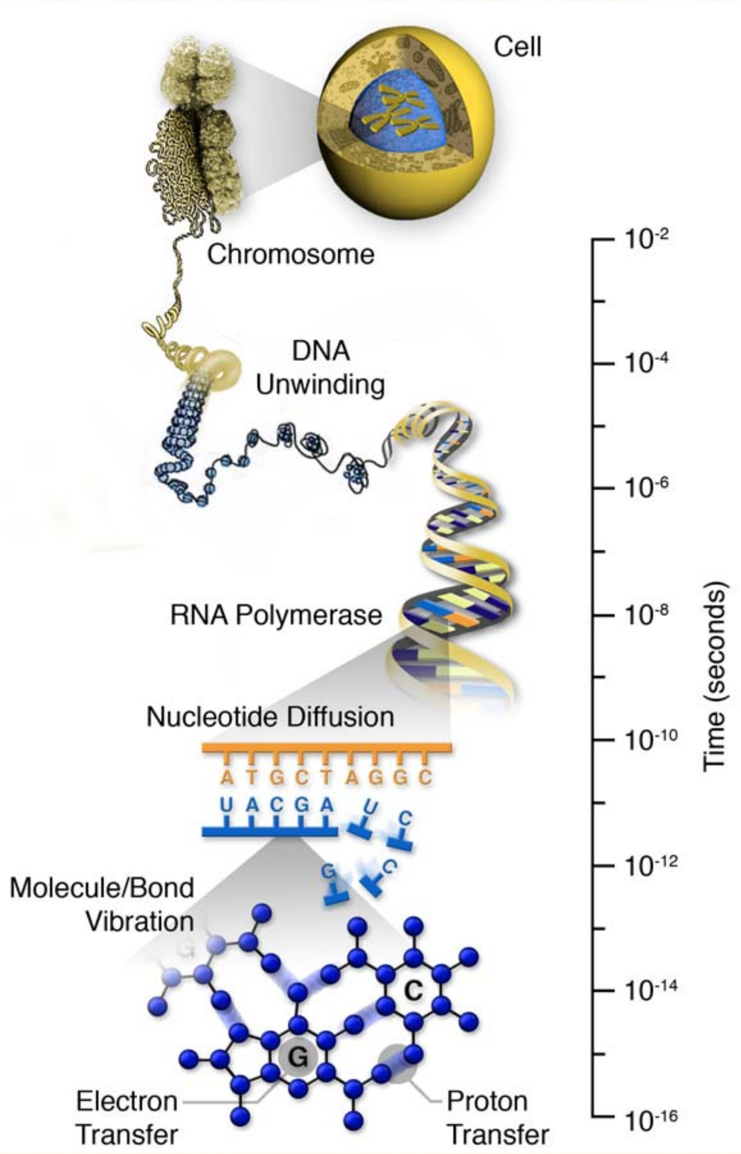
We get the dynamics too!



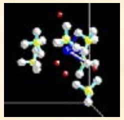
- ● ARCS Fermi Chopper
- ● SEQUOIA Fermi Chopper
- ● HYSPEC
- ● Cold Neutron Chopper Spectrometer
- ● Backscattering
- ● Neutron Spin Echo

We can also measure how things move!

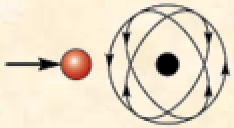
No one length scale, or time scale is more fundamental than any other!



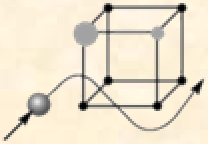
Why Neutrons?



1. Neutrons have the right wavelength



2. Neutrons see the Nuclei



3. Neutrons see Light Atoms next to Heavy Ones

4. Neutrons measure the Velocity of Atoms

5. Neutrons penetrate deep into Matter

6. Neutrons see Elementary Magnets

Neutrons have both Particle-like and Wave-like Properties

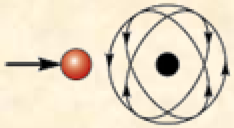
- Mass: $m_n = 1.675 \times 10^{-27}$ kg
- Charge = 0; Spin = ½
- Magnetic dipole moment: $\mu_n = -1.913\ \mu_N$
- Kinetic energy (E), Velocity (v), Wavelength (λ), Wavevector (k)

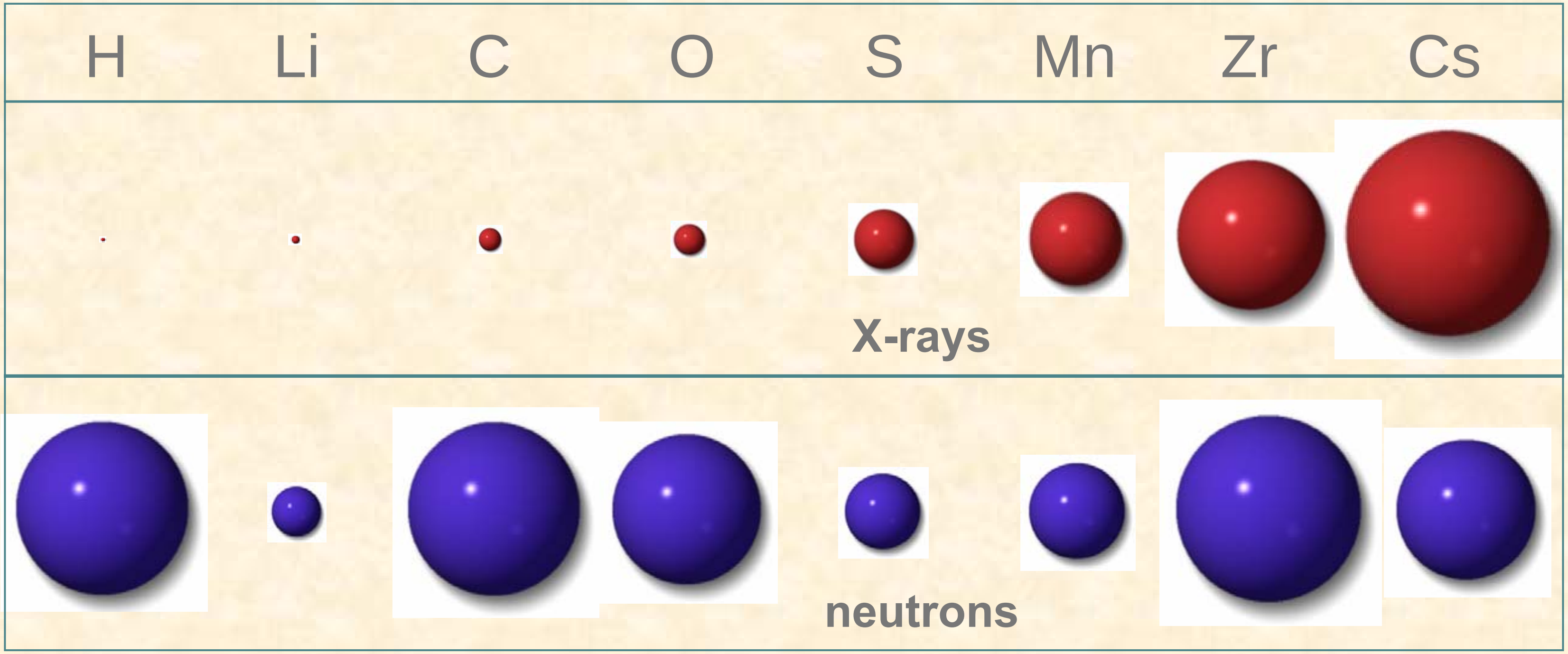
$$E = m_n v^2/2 = k_B T = (hk/2\pi)^2/2\ m_n;\ k = 2\pi/\lambda = m_n v/\ (h/2\pi)$$

	Energy (meV)	Temperature(k)	Wavelength (nm)
Cold	0.1 – 10	1 – 120	0.4 – 3
Thermal	5 – 100	60 – 1000	0.1 – 0.4
Hot	100 - 500	1000 - 6000	0.04 – 0.1

Room temperature ~ 25 meV ~ 0.18 nm ~ 2200 m/s

Neutrons see the Nuclei





How do we produce neutrons?

a. Fission Reactions

$n^1 + U^{235} \longrightarrow$ 2 fission fragments + $2.5n^1$ + 200 MeV

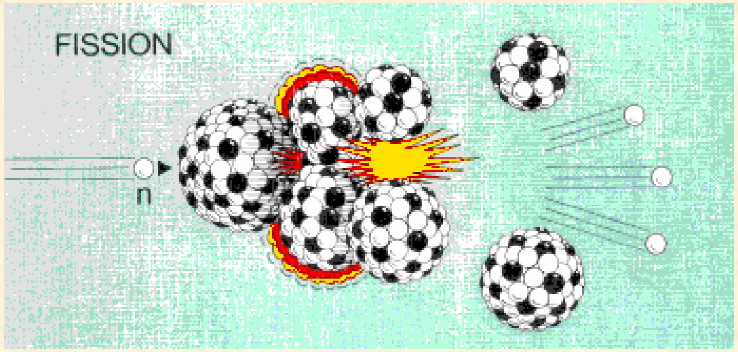
thermal

1 neutron to maintain chain reaction

1 neutron escapes & is available for use

0.5 neutrons absorbed

1 neutron



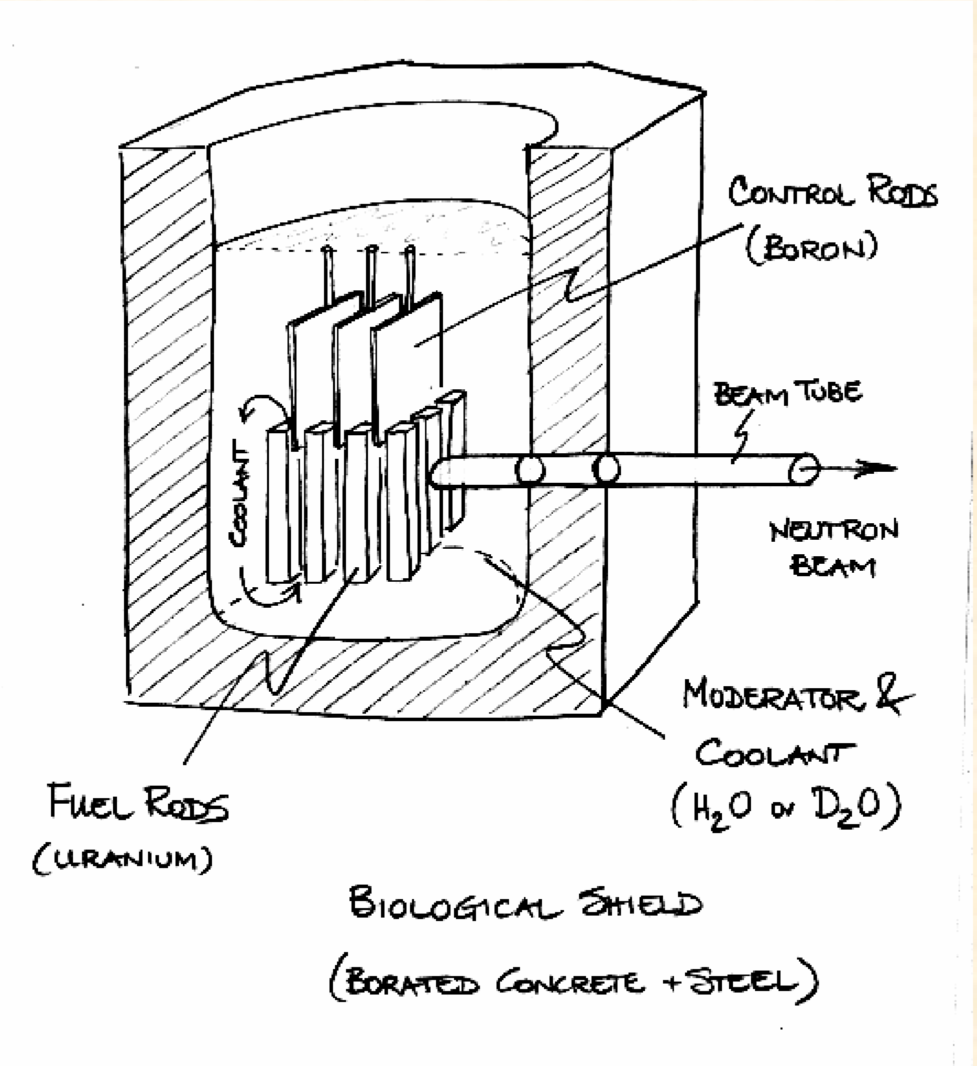
2 to 3 neutrons

Example: 20 MW Research Reactor

$$\text{No. of fissions/sec} = \frac{20 \times 10^6 \text{ watts}}{200 \text{ MeV/fission}} = 6 \times 10^{17} \text{ fissions/second}$$

generates 1.5×10^{18} neutrons/sec in the whole reactor volume

Swimming Pool Reactor

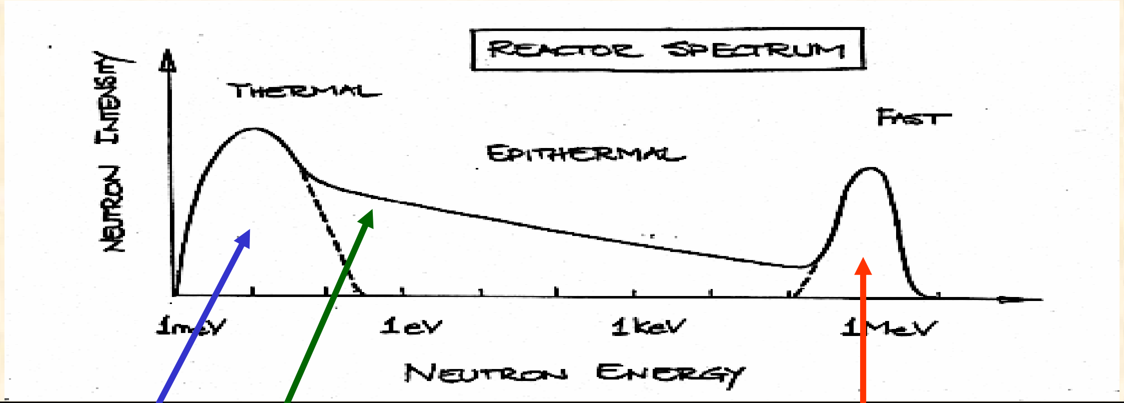


Thermal Neutron Fission

$\nu \sim 2.5$

5×10^{18} fast neutrons/sec generated at 58 MW

Reactor Spectrum



THERMAL E< 200 meV

$$\Phi(E)dE = \Phi_{th}\frac{E}{k_B T}\exp\left(-\frac{E}{k_B T}\right).dE$$

Maxwell-Boltzmann
Region

EPITHERMAL 200 meV < E< 500 keV

$$\Phi(E)dE = \frac{\Phi_{epi}}{E}.dE$$

Slowing Down
or
1/E Region

FAST E > 500 keV & extending to ~ 10 MeV

$$\Phi(E)dE = \Phi_f \exp(-E)\sinh(2E)^{1/2}\,dE$$

Fission Spectrum

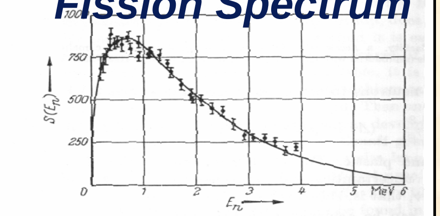


Fig. 2.6.1. The energy spectrum of neutrons produced in thermal neutron fission of U^{235}

Flux Distribution around ILL Core

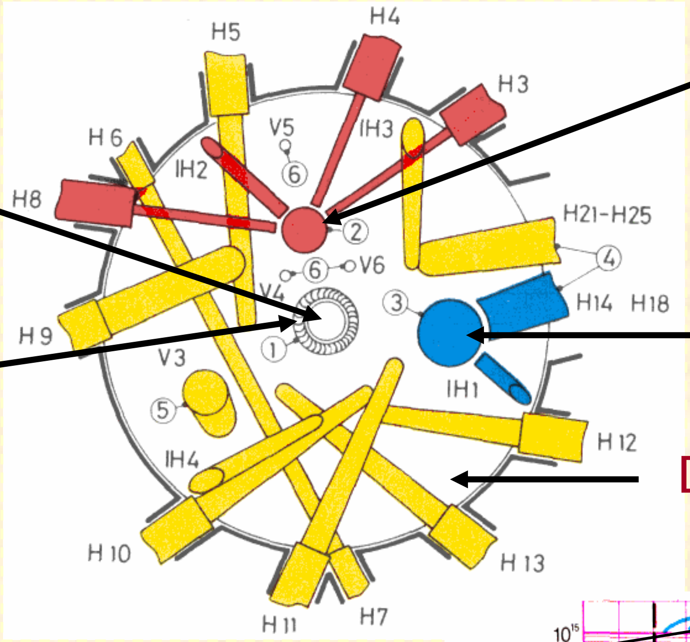
Control Rod

Hot Source

Cold Source

Fuel Element

D_2O Reflector



58MW 93% U^{235}

Thermal

$1.2\ 10^{15}$ n/cm²/s

Epithermal

$8\ 10^{13}$ n/cm2/s

Fast

$2.5\ 10^{14}$ n/cm2/s

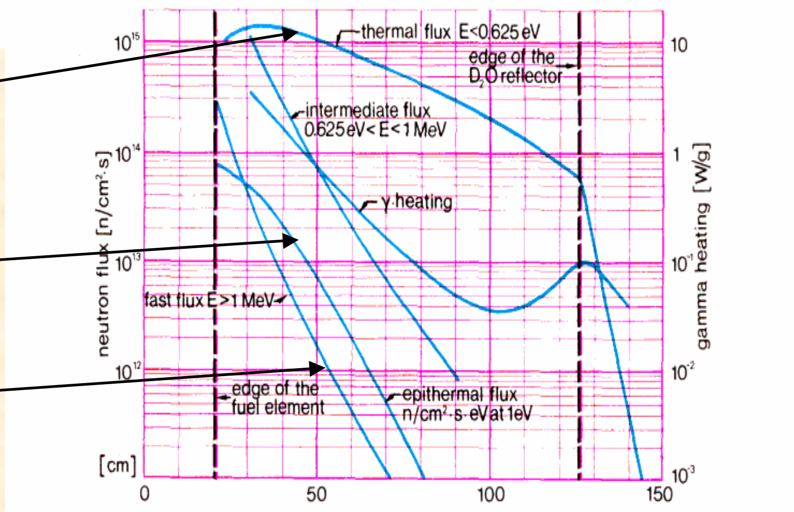
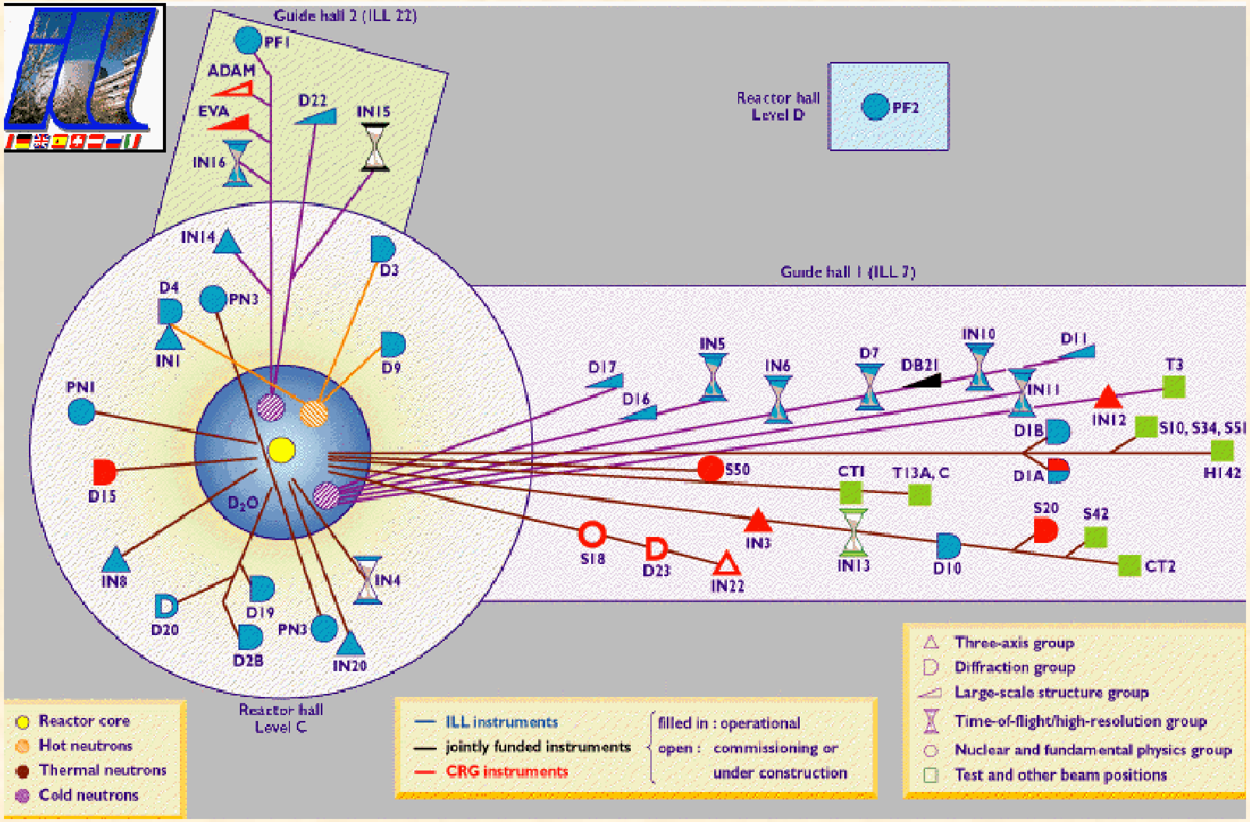


Fig. 2. Local flux distribution of the HFR as a function of the distance from the core axis.

ILL Instrument Layout

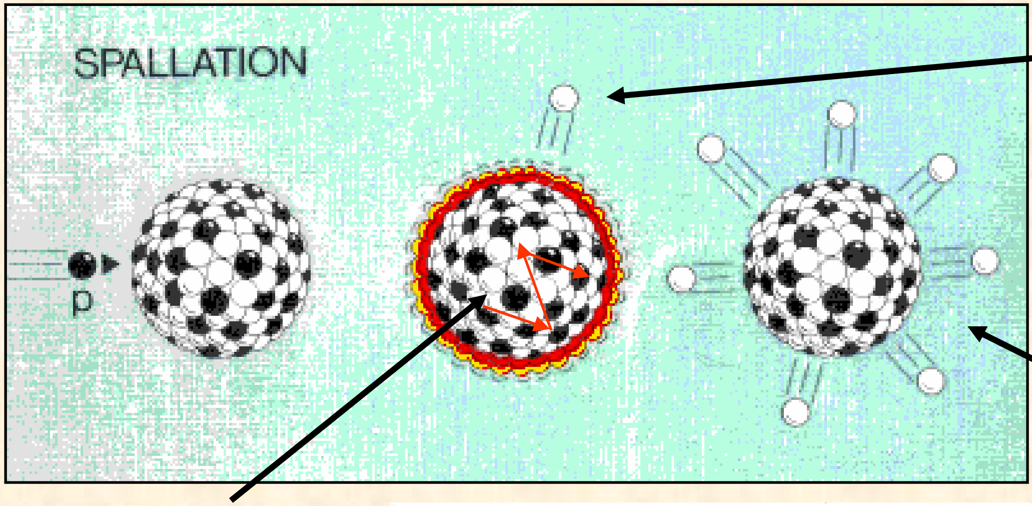


~40 instruments operating:	12 diffractometers
	12 spectrometers
	6 nuclear physics
	10 special instruments

How do we produce neutrons?

b. Artificially accelerated particles

(iii) Spallation with Protons

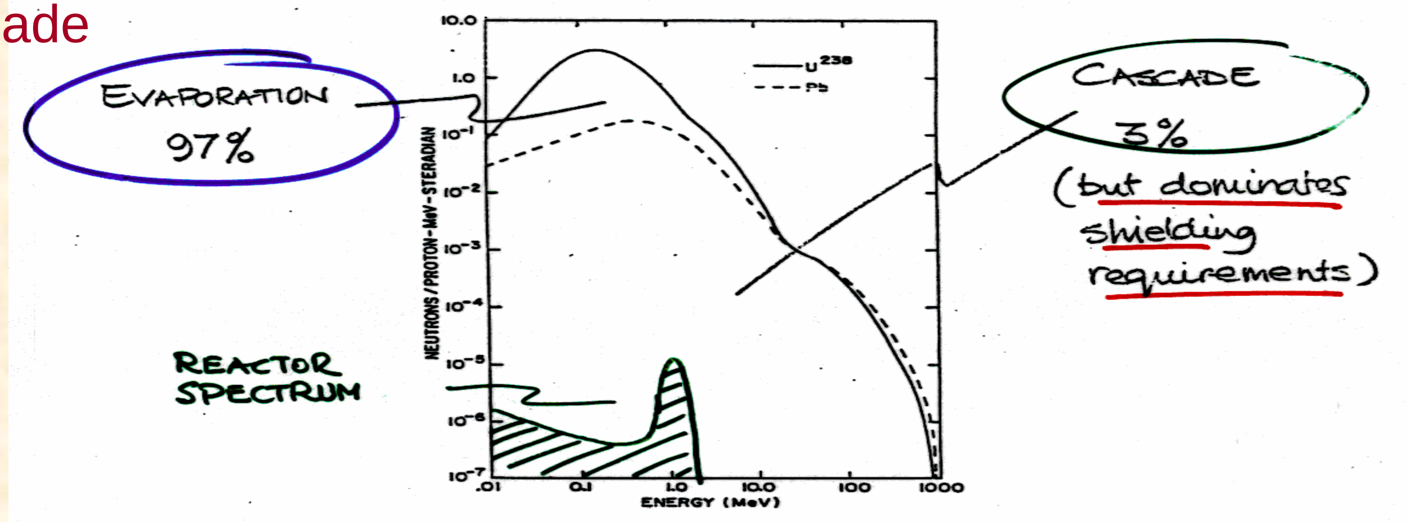


2. Inter Nuclear Cascade

3. Evaporation

1. Internal Cascade

Up to 40 neutrons per incident proton

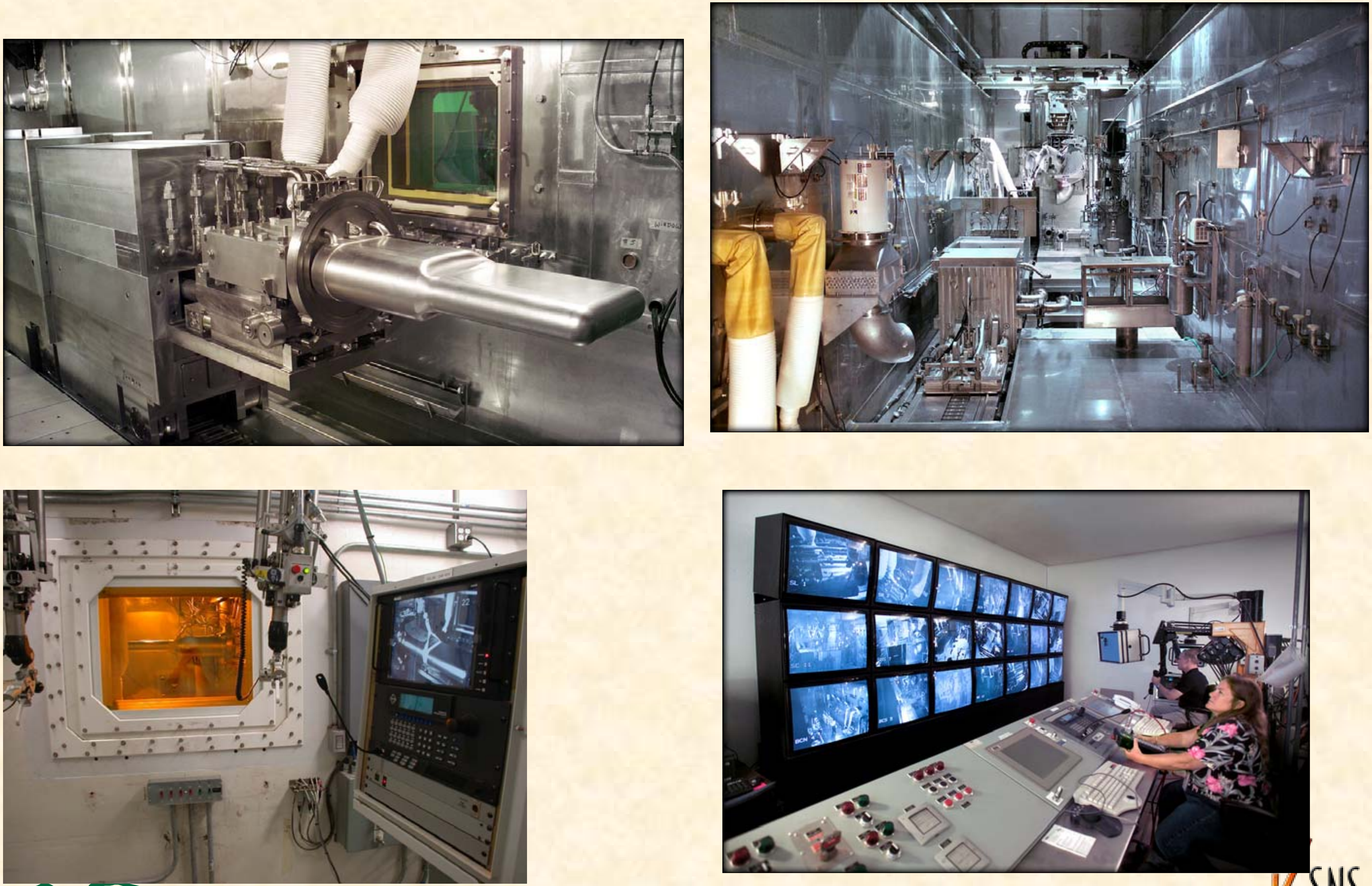


The Spallation Neutron Source

- Construction completed May 2006
- Room for eventual 25 instruments spanning physics, chemistry, biology, & materials science
- SNS will become the world's leading facility for neutron scattering
- Upgradeable to higher power, 2nd target

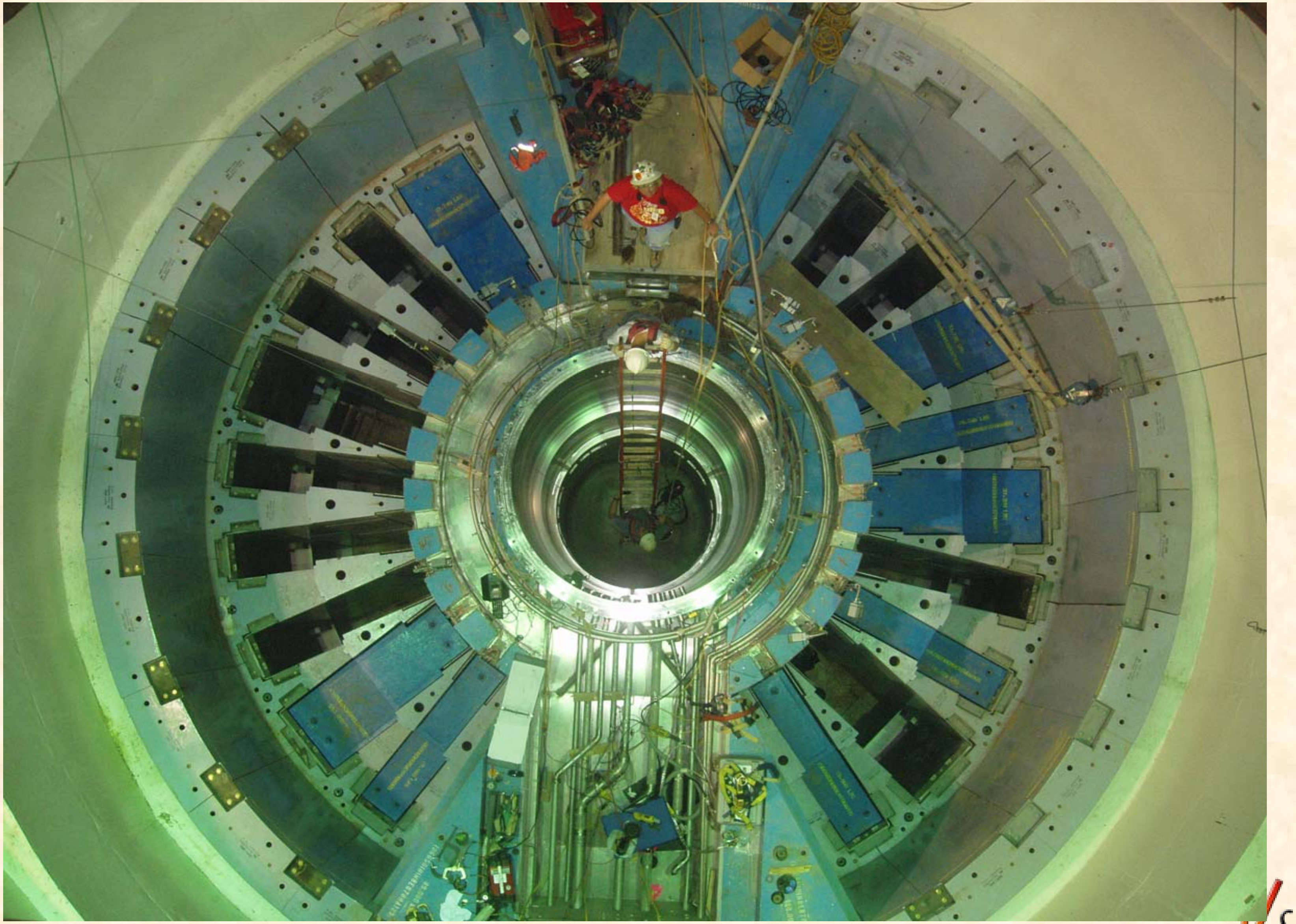
Linear Accelerator

Mercury Target

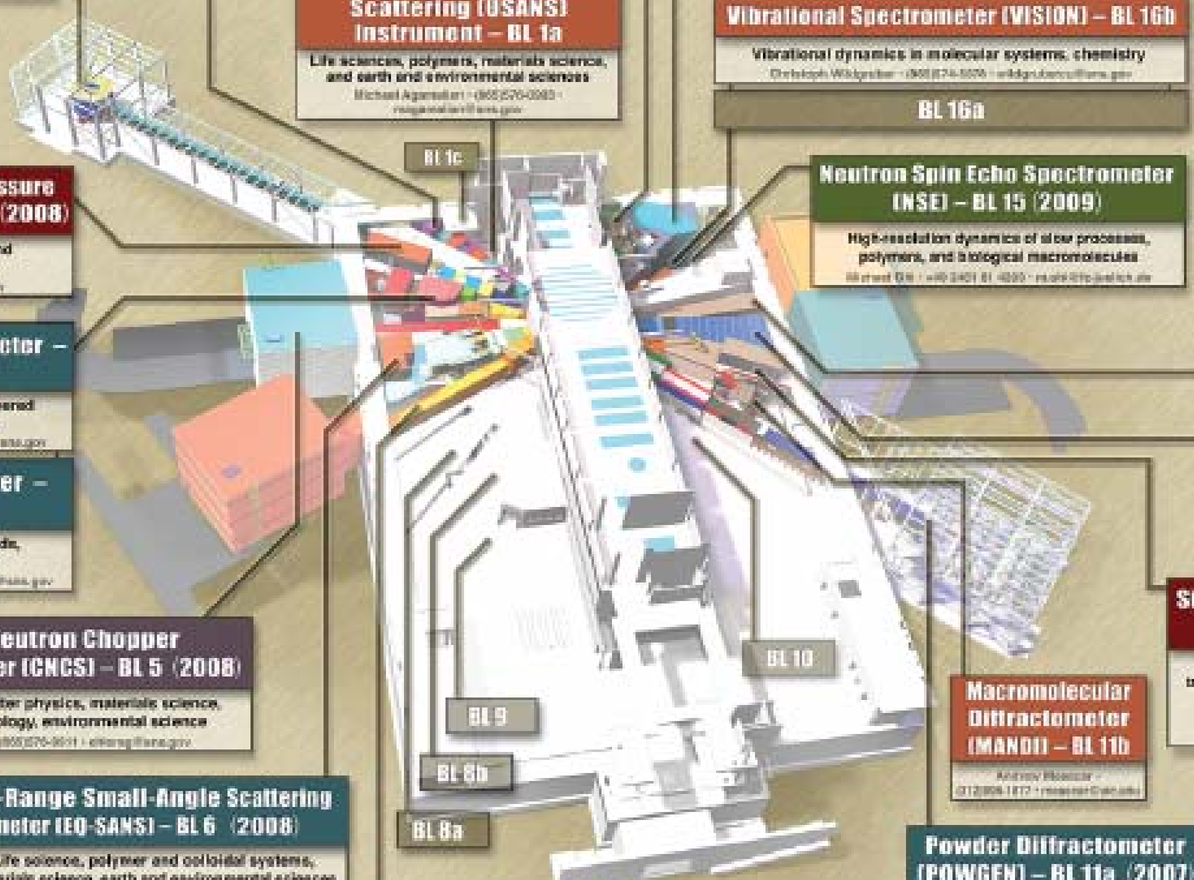


You can teach the robots anything….

Monolith – October 2004



Spallation Neutron Source



Backscattering Spectrometer – BL 2 (2006*)

Dynamics of macromolecules, constrained molecular systems, polymers, biology, chemistry, materials science

Ken Herwig · (865)576-2065 · herwigkw@ornl.gov

Nanoscale-Ordered Materials Diffractometer (NOMAD) – BL 1b (2011)

Liquids, glasses, polymers and biological macromolecular systems, partially ordered complex materials

Joerg Neuefeind · (865)241-1836 · neuefeindjc@ornl.gov

Wide Angular-Range Chopper Spectrometer (ARCS) – BL 18 (2007)

Atomic-level dynamics in materials science, chemistry, condensed matter sciences

Doug Abernathy · (865)576-5105 · abernathydl@ornl.gov

Fine-Resolution Fermi Chopper Spectrometer (SEQUOIA) – BL 17 (2009)

Dynamics of complex fluids, quantum fluids, magnetism, condensed matter, materials science

Garrett Granroth · (865)576-0900 · granrothge@ornl.gov

Ultrasmall-Angle Neutron Scattering (USANS) Instrument – BL 1a

Life sciences, polymers, materials science, and earth and environmental sciences

Michael Agamalian · (865)576-0283 · agamalianm@ornl.gov

Vibrational Spectrometer (VISION) – BL 16b

Vibrational dynamics in molecular systems, chemistry

Christoph Wildgruber · (865)574-5076 · wildgruberc@ornl.gov

BL 16a

Spallation Neutrons and Pressure Diffractometer (SNAP) – BL 3 (2008)

Materials science, geology, earth and environmental sciences

Chris Tulk · (865)576-7028 · tulkca@ornl.gov

Neutron Spin Echo Spectrometer (NSE) – BL 15 (2009)

High-resolution dynamics of slow processes, polymers, and biological macromolecules

Michael Ohl · +49 2461 61 4203 · m.ohl@fz-juelich.de

Hybrid Chopper Spectrometer (HYSPEC) – BL 14B (2011)

Atomic-level dynamics in single crystals, magnetism, condensed matter sciences

Mark Hagen · (865)241-8481 · hagenme@ornl.gov

BL 14a

Magnetism Reflectometer – BL 4a (2006)

Chemistry, magnetism of layered systems and interfaces

Frank Klose · (865)576-5099 · klosefr@ornl.gov

Liquids Reflectometer – BL 4b (2006)

Interfaces in complex fluids, polymers, chemistry

John Ankner · (865)576-5122 · anknerjf@ornl.gov

Fundamental Physics Beam Line – BL 13 (2008)

Fundamental properties of neutrons

Geoffrey Greene · (865)574-0436 · greenegl@ornl.gov

Single-Crystal Diffractometer (TOPAZ) – BL 12 (2009)

Atomic-level structures in chemistry, biology, earth science, materials science, condensed matter physics

Christina Hoffmann · (865)576-5127 · hoffmanncm@ornl.gov

Cold Neutron Chopper Spectrometer (CNCS) – BL 5 (2008)

Condensed matter physics, materials science, chemistry, biology, environmental science

Georg Ehlers · (865)576-0611 · ehlersg@ornl.gov

Macromolecular Diffractometer (MANDI) – BL 11b

Andrew Mesecar · (312)996-1877 · mesecar@uic.edu

Extended Q-Range Small-Angle Scattering Diffractometer (EQ-SANS) – BL 6 (2008)

Life science, polymer and colloidal systems, materials science, earth and environmental sciences

Jinkui Zhao · (865)574-0411 · zhaoj@ornl.gov

Powder Diffractometer (POWGEN) – BL 11a (2007)

Atomic-level structures in magnetism, chemistry, materials sciences

Jason Hodges · (865)576-7034 · hodgesjp@ornl.gov

Engineering Materials Diffractometer (VULCAN) – BL 7 (2008)

Engineering, materials science, materials processing

Xun-Li Wang · (865)576-8184 · wangxl@ornl.gov

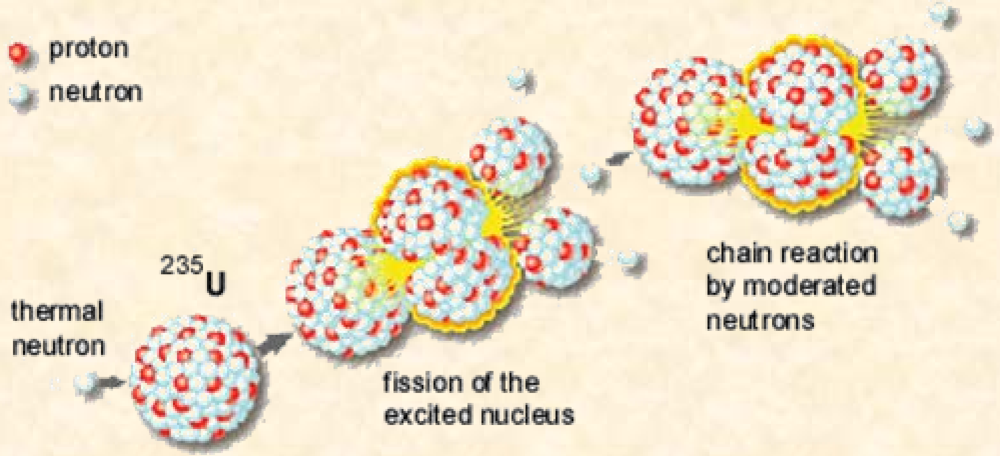
* Date shown is the scheduled commissioning date.

LEGEND

🟦	SNS TPC	🟥	SNS 1	🟧	SNS 2
🟪	DOE Grant	🟫	DOE NP	🟩	Non U.S.

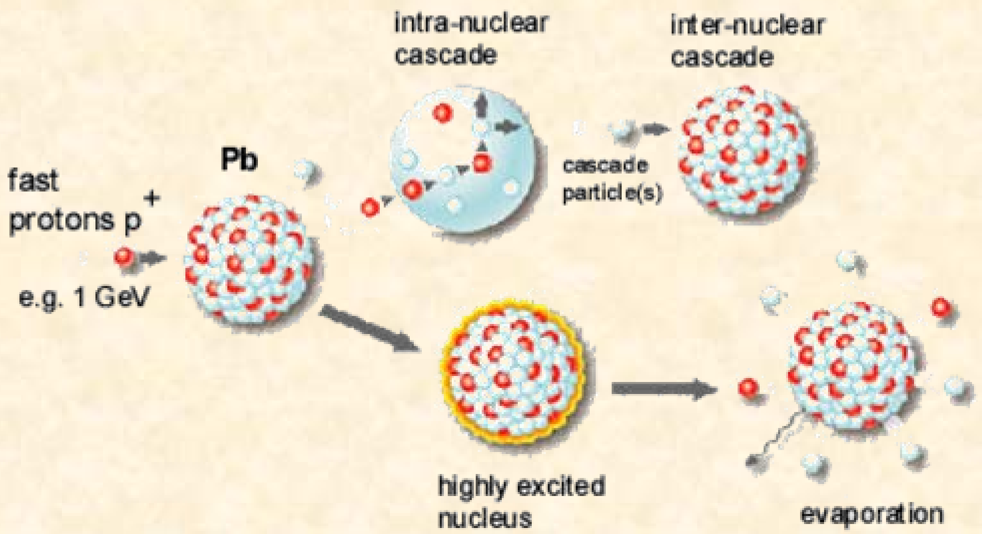
06-G00460/arm

How do we produce neutrons?



Fission

- chain reaction
- continuous flow
- 1 neutron/fission
- 180 MeV/neutron

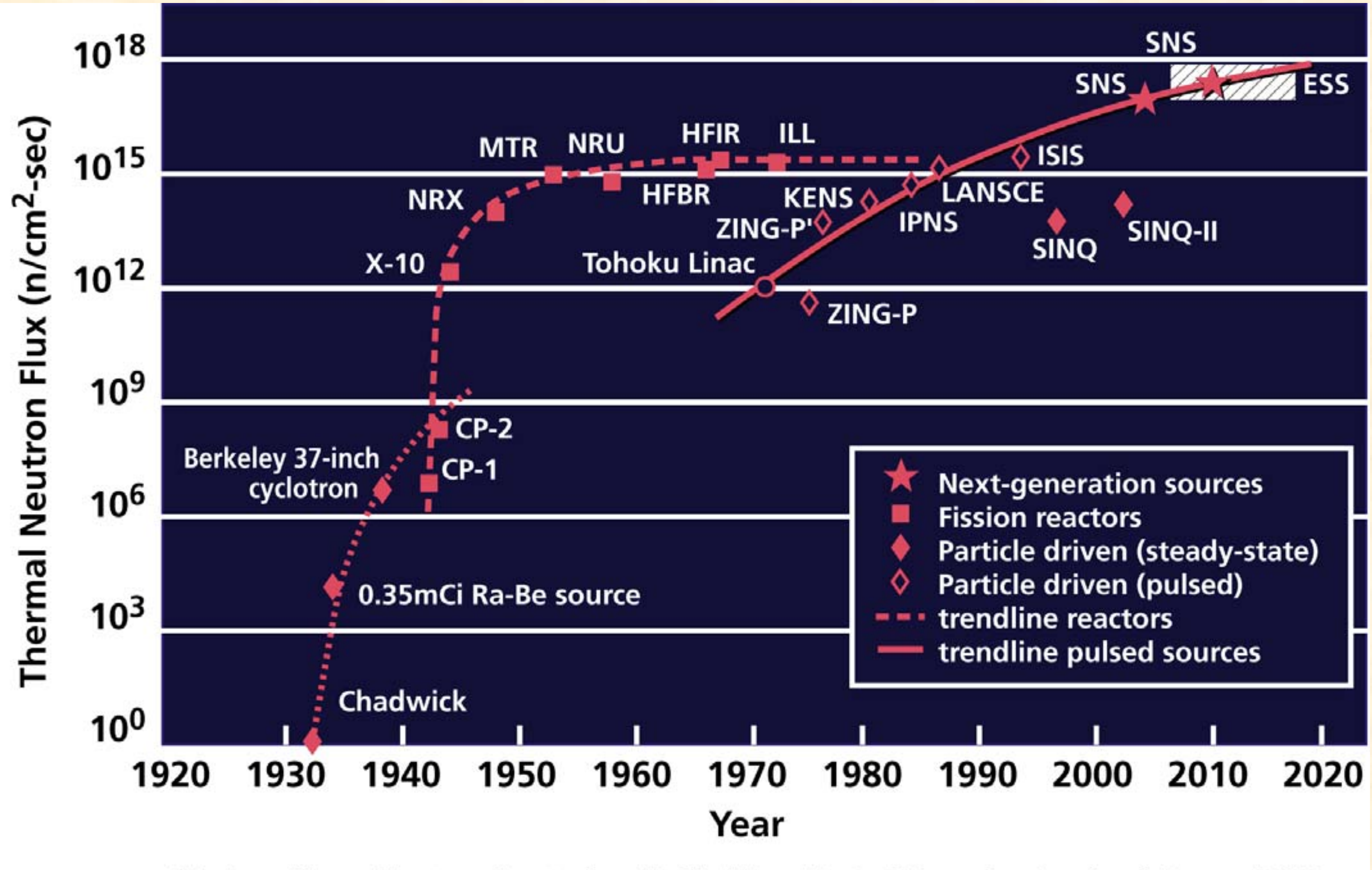


Spallation

- no chain reaction
- pulsed operation
- 40 neutrons/proton
- 30 MeV/neutron

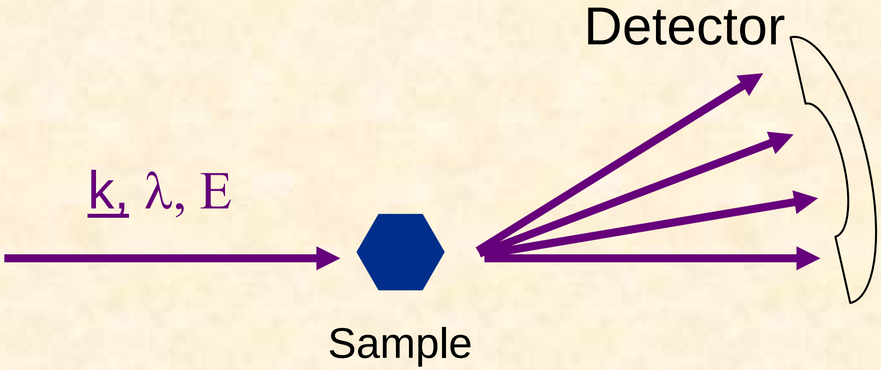
Higher neutron Fluxes?

Reactors have reached the limit at which heat can be removed from the core
Pulsed sources have not yet reached that limit and hold out the promise of higher intensities



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

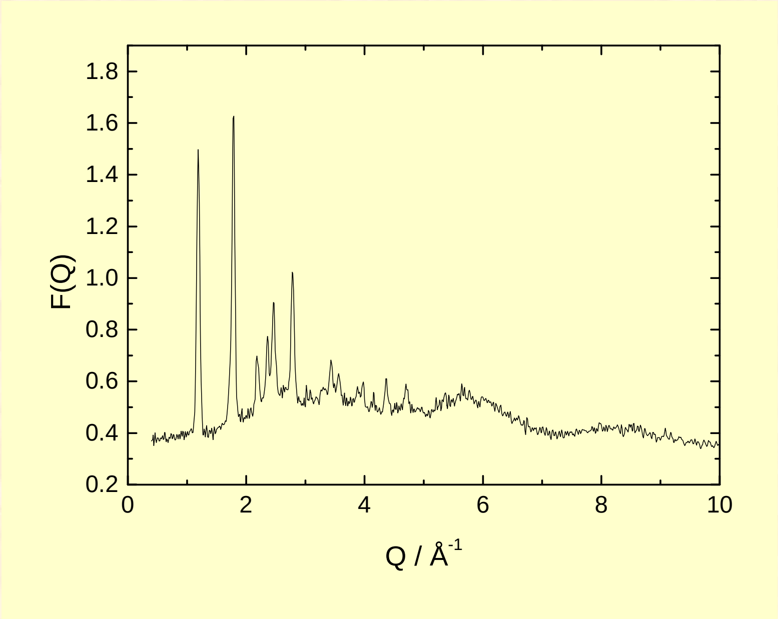
What do we measure?

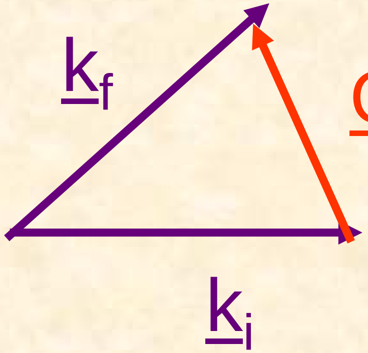


Detector

$\underline{k}$, λ, E

Sample





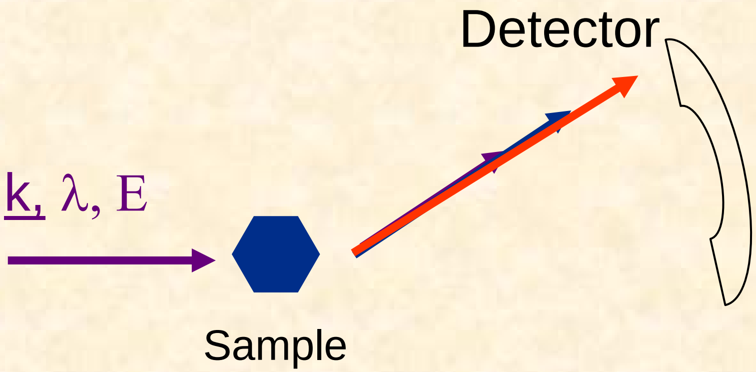
$\underline{k}_f$

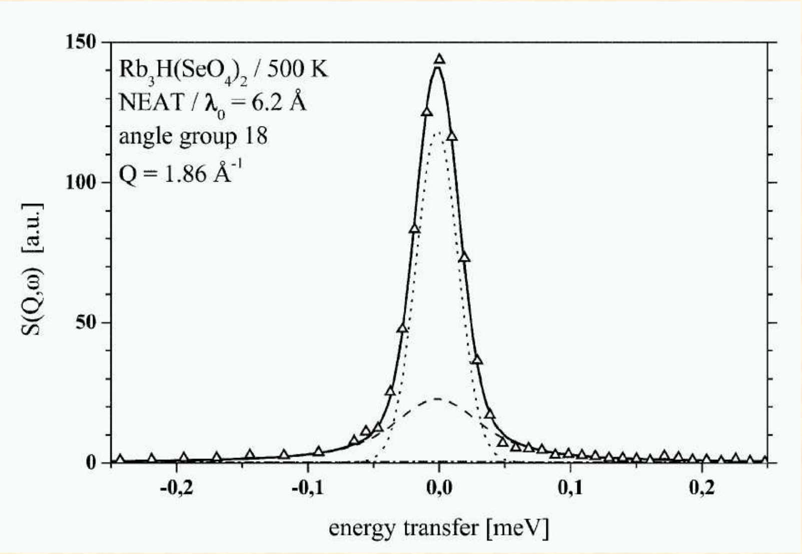
$\underline{k}_i$

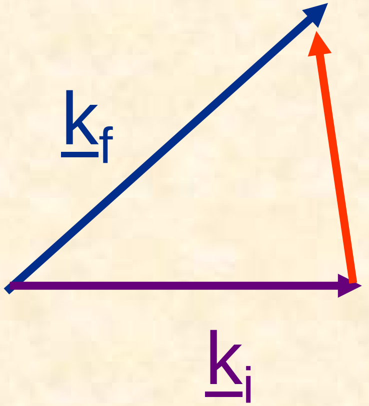
$\underline{Q} = \underline{k}_f - \underline{k}_i$ Wavevector transfer

$|k_f| = |k_i|$ “Elastic” scattering $I(\underline{Q})$

What do we measure?







$\underline{Q} = \underline{k}_f - \underline{k}_i$ Wavevector transfer

$\hbar\omega = \underline{E}_f - \underline{E}_i$ Energy transfer

$|k_f| \neq |k_i|$ "Inelastic" scattering $I(\underline{Q}, \omega)$

What information do we get?

$$I(\vec{Q},\omega) = b_{coh}^{2}\frac{k'}{k}NS(\vec{Q},\omega)$$

$$S(\vec{Q},\omega) = \frac{1}{h}\iint G(\vec{r},t)e^{i(\vec{Q}.\vec{r}-\omega t)}d\vec{r}dt$$

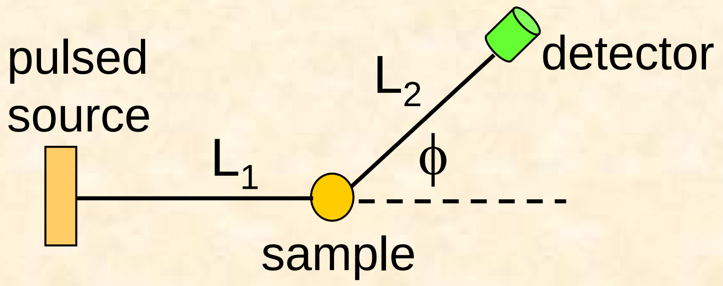
$$S_i(\vec{Q},\omega) = \frac{1}{h}\iint G_s(\vec{r},t)e^{i(\vec{Q}.\vec{r}-\omega t)}d\vec{r}dt$$

Inelastic coherent scattering measures correlated motions of atoms

Inelastic incoherent scattering measures self-correlations, e.g., diffusion

Determining the Wavelength

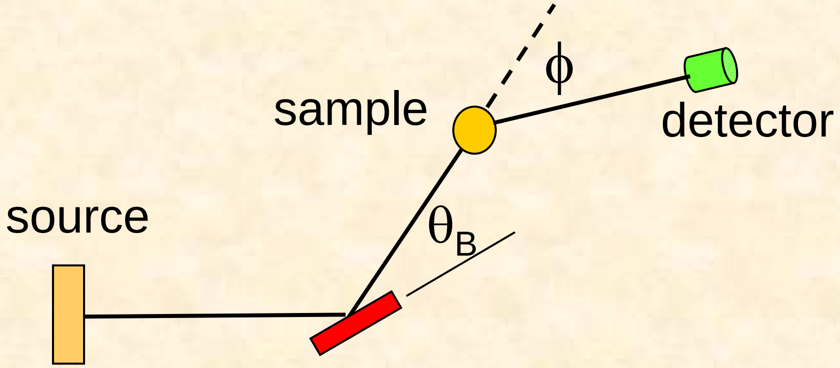
time-of-flight (TOF)



$$\lambda = \frac{4000}{v} = \frac{4000\,(t-t_0)}{L}$$

$$\delta\lambda \sim \delta t_0,\ \delta t,\ \delta L$$

crystal monochromator (Bragg diffraction)

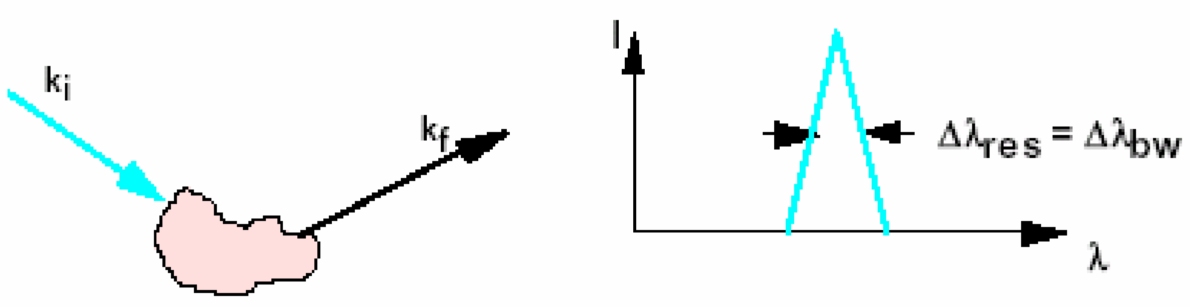


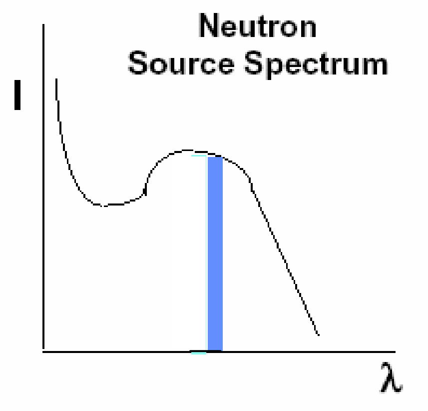
$$\lambda = \frac{2d_c \sin(\theta_B)}{n}$$

$$\delta\lambda \sim \delta d_c,\ \delta\theta_B$$

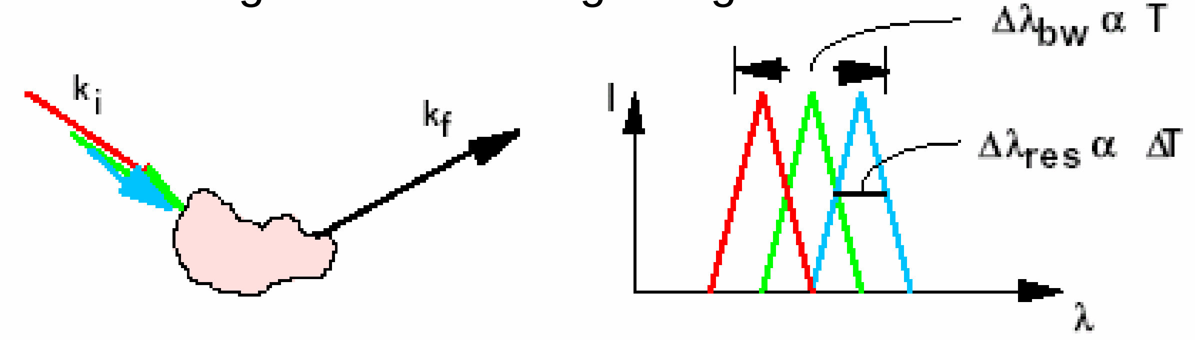
Differences between TOF and steady-state

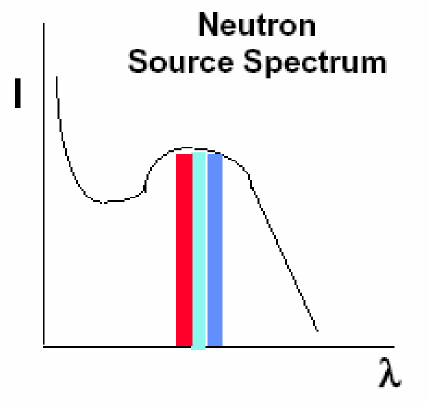
Steady-state
- uses single wavelength
- bandwidth (bw) = resolution width (res)
- range of data requires multiple angles





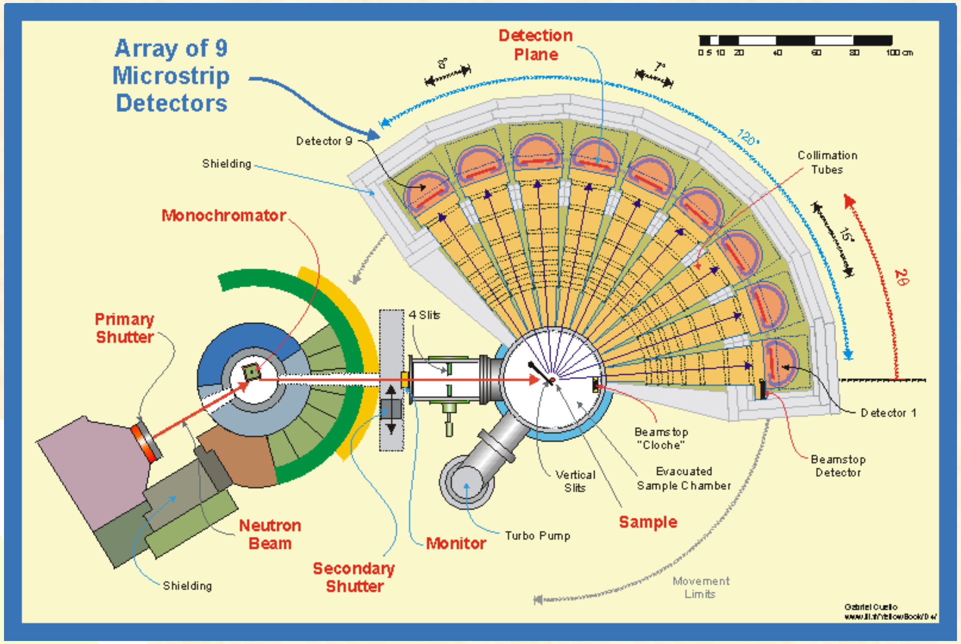
TOF
- uses range of wavelengths
- bandwidth (bw) >> resolution width (res)
- range of data at single angle



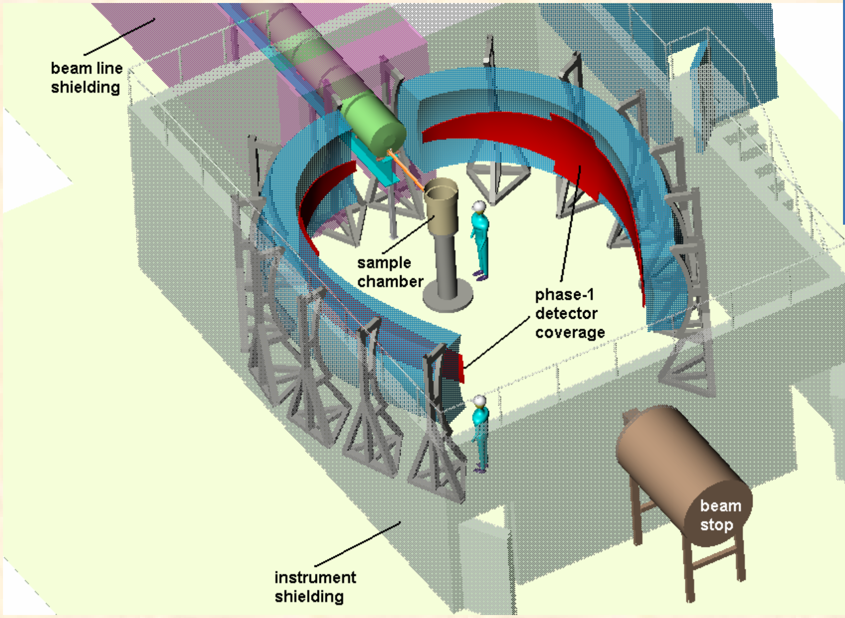


Diffraction instruments

Reactor

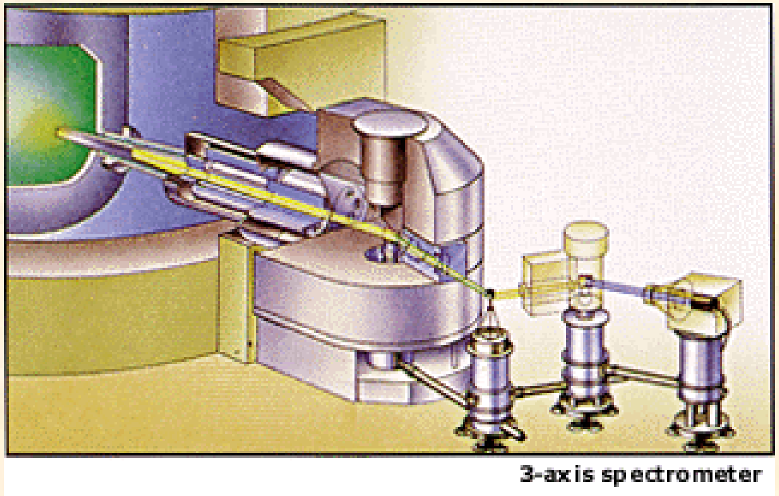


Gabriel Cuello
www.ill.fr/YellowBook/D4/



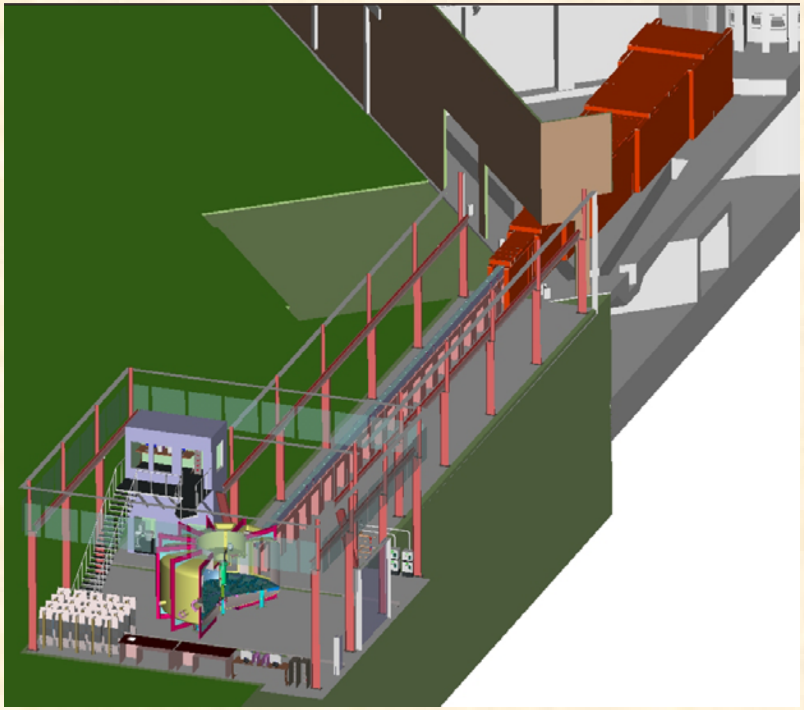
Spallation source

Inelastic instruments

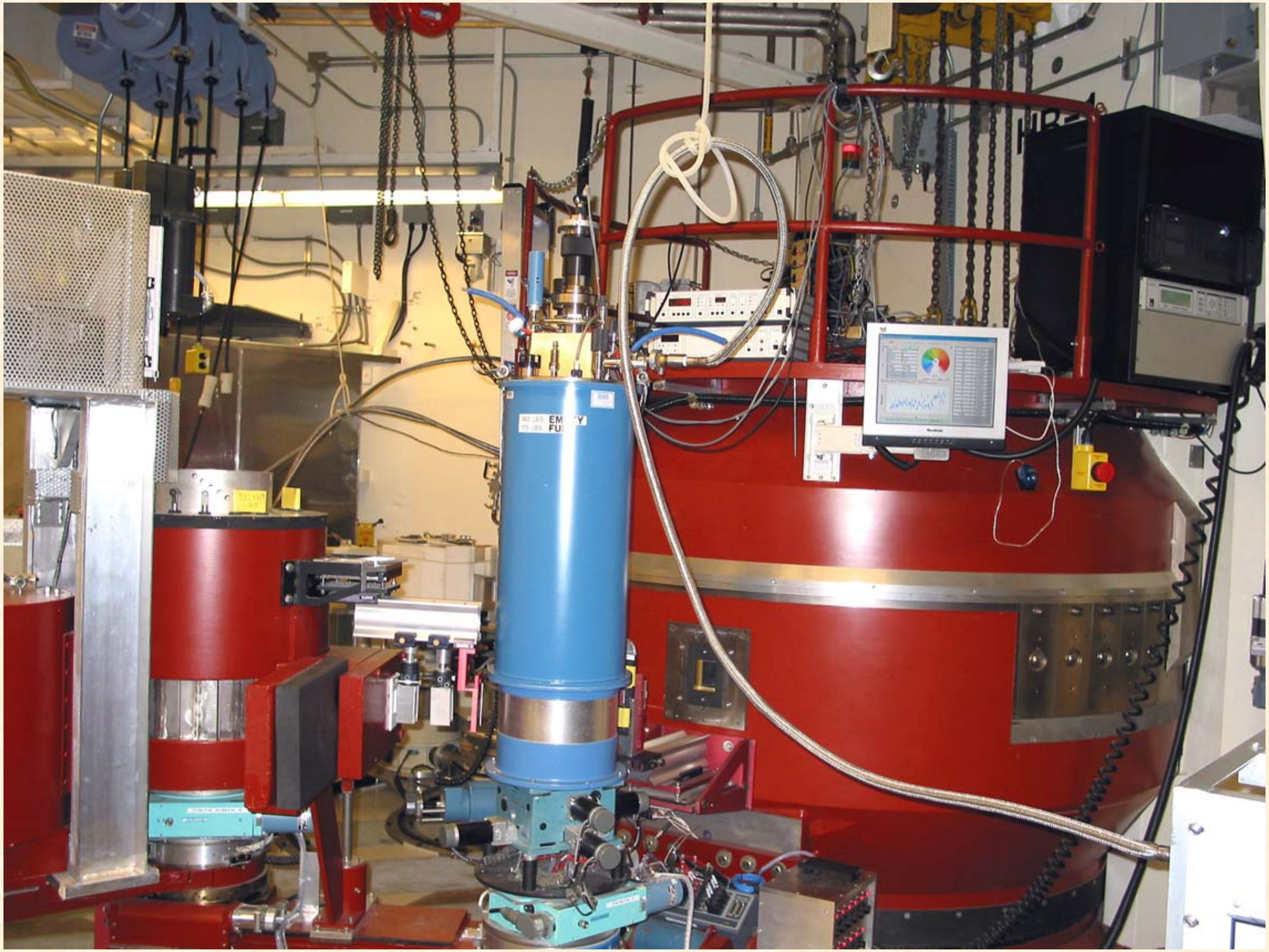


Reactor

Spallation source



Triple Axis Instrument at HFIR



SNS Backscattering Spectrometer

Major Facilities in North America

The North American Neutron Scattering Centers

1

NRC CNRC

Beam Time

Proposals for experiments at the Canadian Neutron Beam Centre are accepted and scheduled on a continuing basis. Upon receipt of the proposals, a local scientific contact is assigned to the experiment if none is specified on the proposal. The proposal is then reviewed by a formal committee for scientific merit, technical feasibility, and duration. Accepted proposals are scheduled by CNBC staff. Please see our website for more details.

Contact
http://neutron.nrc.gc.ca

The Canadian Neutron Beam Centre

The NRU Reactor

The NRU reactor at Chalk River is rated at 135 MW with a peak thermal flux of 3 X 10^{18} neutrons/m^2/s. Heavy water is used for moderation and cooling. The reactor can be continuously refueled while operating to minimize downtime. The spectrometers operate approximately 80% of the year. Five thermal neutron spectrometers are currently operating with two more under construction.

Canada

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The Intense Pulsed Neutron Source (IPNS) at Argonne National Laboratory

IPNS Instrument Suite

- Co-located at Argonne National Laboratory with the Advanced Photon Source (APS) and other user facilities for materials characterization
- Operating continuously since 1981 as a US Department of Energy National User Facility, with users representing universities, industrial corporations, and government-sponsored research laboratories throughout the US and overseas.

Further background along with contact information found at
www.pns.anl.gov

- Instruments:
  HRMECS - High-Resolution Medium-Energy Chopper Spectrometer
  QENS - Quasielastic Neutron Spectrometer
  GLAD - Glass, Liquids and Amorphous Materials Diffractometer
  SCD - Single-Crystal Diffractometer
  SEPD - Special Environment Powder Diffractometer
  LRMECS - Low-Resolution Medium-Energy Chopper Spectrometer
  SAND - Small Angle Neutron Diffractometer
  POSY II - Unpolarized Neutron Reflectometer
  POSY I - Polarized Neutron Reflectometer
  SASI - Small Angle Scattering Instrument
  HIPD - High-Intensity Powder Diffractometer
  GPPD - General-Purpose Powder Diffractometer
  Corelli - Correlation Chopper Diffuse Scattering Diffractometer

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The Los Alamos Neutron Science Center (LANSCE): Serving Over 500 Users Annually

LANSCE provides a versatile array of capabilities for researchers who use neutrons and protons in basic and applied research. Neutron energies available range from meV to hundreds of MeV.

- The Manuel Lujan Neutron Scattering Center provides a suite of 14 instruments for research in condensed matter science, materials properties, structural biology, and nuclear science. The Lujan Center focuses its attention on the development of instruments and methods for addressing problems that are of interest to both the basic research community and the nation's Nuclear Stockpile Stewardship Program. Examples include the study of elastic strain in metals and composites; the determination of bulk texture; structural studies at high pressure; characterization of the morphology of polymers and blends; and the examination of the structure of protective layers, coatings, and adhesives.
- At the proton radiography facility (pRad), scientists use protons to photograph detonation waves, a science-based rather than test-based approach to stockpile stewardship. Proton radiography offers several advantages over conventional x-ray techniques for radiographing thick, dense, dynamic systems.
- The Weapons Neutron Research Facility (WNR) uses protons and unmoderated neutrons for research in areas such as nuclear structure, fission cross sections, neutron-induced reactions, neutron resonance spectroscopy, and neutron-induced failures in semiconductor devices. WNR utilizes two target areas and their associated flight paths.
- LANSCE'S new Isotope Production Facility (IPF) was completed in early 2004 to provide radioisotopes for medicine, industry, and research nationwide. The IPF utilizes a 100-MeV proton beam extracted from the LANSCE accelerator. Some isotopes, such as aluminum-26 and silicon-32, are unique to LANSCE.

To learn about the instruments and capabilities of LANSCE, to become a member of the LANSCE User Group, or to submit a proposal for beam time, *please visit our website at*
lansce.lanl.gov

Los Alamos National Laboratory

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NIST CENTER FOR NEUTRON RESEARCH, North America's major source for cold neutrons

THERMAL NEUTRON INSTRUMENTS

Proposals welcome from around the world. Please go to our website:
www.ncnr.nist.gov/call/current_call.html

COLD NEUTRON INSTRUMENTS

1. MACS, triple axis spectrometer with double focusing monochromator and multiple crystal analyzer/detectors (under construction)
11. NG-7 Horizontal Sample Reflectometer
12. Neutron Interferometry and Optics Station
13. Spin-Polarized Triple Axis Spectrometer (SPINS) – part of NSF/NIST Center for High Resolution Neutron Scattering (CHRNS)
14. Spin Echo Spectrometer – part of CHRNS
15. Prompt Gamma Activation Analysis (PGAA)/Neutron Depth Profiling
16. NG-7 30-m Small Angle Neutron Scattering (SANS)
17. Neutron Physics Station
18. Fermi Chopper hybrid time-of-flight (TOF) Spectrometer
19. Disk Chopper TOF Spectrometer – part of CHRNS
20. NG-3 30-m SANS – part of CHRNS
21. Backscattering Spectrometer – part of CHRNS
22. NG-1 10-m SANS (under construction) replacing the current 8-m SANS
23. Vertical Sample Reflectometer
24. Advanced Neutron Diffractometer/Reflectometer (AND/R) – part of the Cold Neutrons for Biology and Technology program

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High Flux Isotope Reactor (HFIR) Center for Neutron Scattering

OAK RIDGE NATIONAL LABORATORY

The HFIR Center for Neutron Scattering at the Oak Ridge National Laboratory is the highest flux reactor-based source of neutrons for condensed matter research in the United States. The Center is a national user facility operated by ORNL for the U.S. Department of Energy. Thermal and cold neutrons produced by the HFIR are used to study physics, chemistry, materials science, engineering, and biology.

For more information on submitting a proposal, instrumentation, or scientific contacts, please visit our web site at neutrons.ornl.gov.

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Spallation Neutron Source at Oak Ridge National Laboratory

- A 1.4-MW spallation source funded by the U.S. Department of Energy will come into operation in June 2006
- 17 of 24 instruments approved; 16 under various stages of construction
- Adjacent to the Center for Nanophase Materials Sciences

For additional information, visit
http://www.sns.gov


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