Neutron Instrumentation Part 1: Basics

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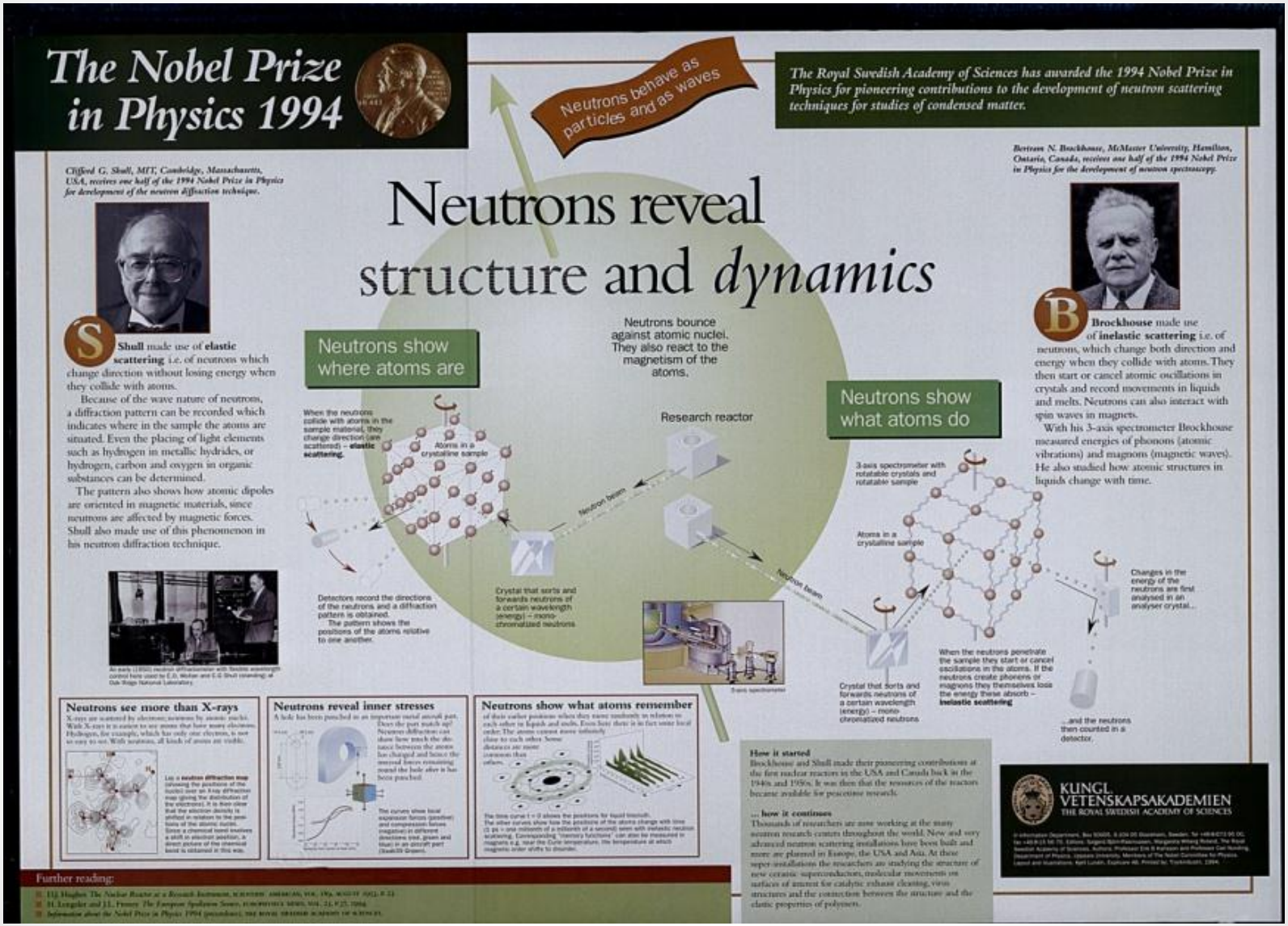
Ian Anderson

What we will cover in Part 1

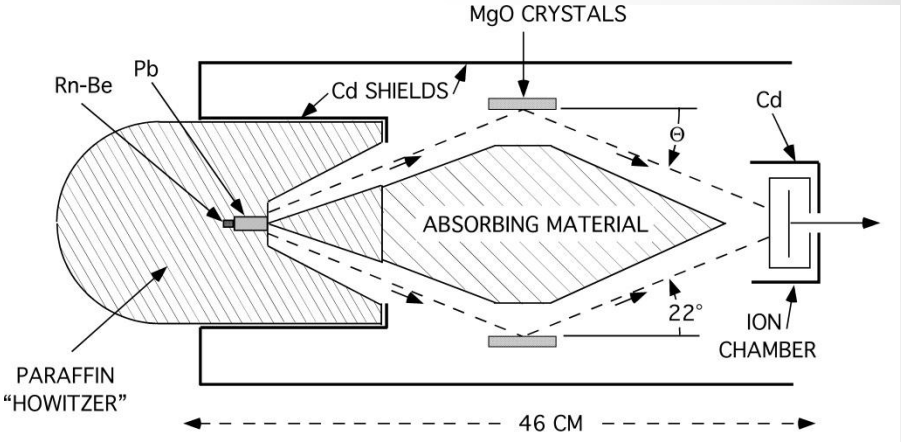
- Some history
- Properties of the neutron
- What do we measure
- Liouville's theorem

Why neutrons?



In the beginning....

1932 Chadwick
1936 Demonstrations of neutron Bragg scattering
1942 CP1 goes critical in Stagg Field, Chicago – First Nuclear Reactor
1942 Roosevelt orders the Manhattan Project.
1943 November, ORGR goes critical
1943 CP-1 was moved to Argonne Woods and started up as CP-2.
1944 CP-3, the D2O reactor, goes critical
1945 E. Wollan installs first two axis diffraction instrument (x-ray) at ORGR, and W. Zinn a similar instrument at CP-3
1945 Early expts on xstals (Shull and Wollan), (Fermi and Zinn)
1946 First powder diffraction measurements made on NaCl and single crystal experiments
1946 – 1948 systematic investigation of the fundamentals of neutron scattering (published 1948)
1948 First Laue and radiography
1948 NaCl monochromators replaced by metal crystals
1949 Determination of the structure of ice (Pauli model) led to work on structure of ThH2 and ZrH2 (Rundle 1952)
1950 First custom built 2-axis diffractometer installed at ORGR
1951 First structure refinement from neuton diffraction (Peterson and Levy)
1951 First published results on magnetic scattering ->distinction between Bloch and Schwinger models for neutron magnetic interaction



Mitchell, D. P., and P. N. Powers (1936) Bragg reflection of slow neutrons, Phys. Rev. 50, 486.

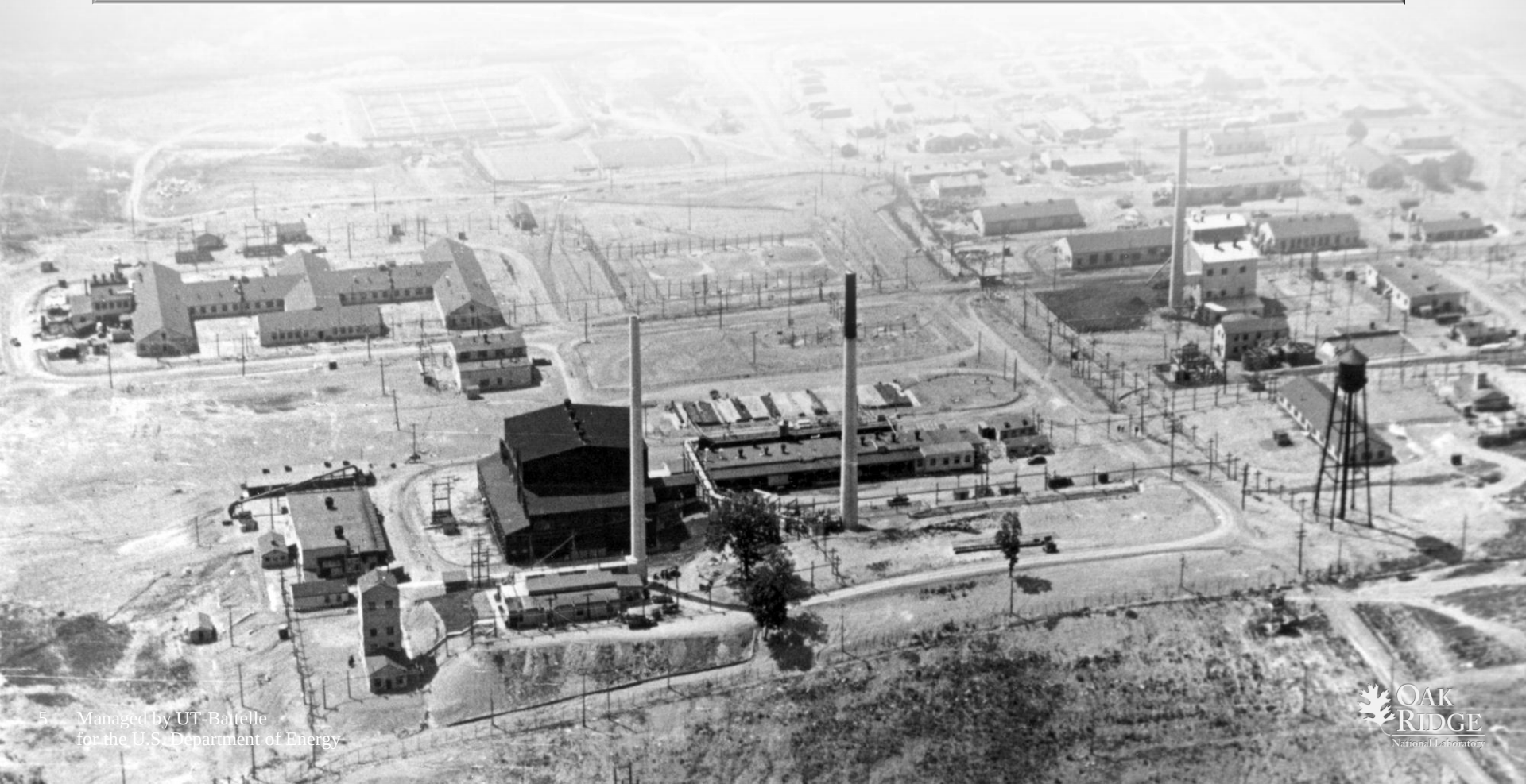
von Halban, H., and P. Preiswerk (1936). Preuve expérimentale de la diffraction des neutrons: Experimental proof of neutron diffraction, Comptes Rendus, 203, 73 .

Preiswerk, P. (1937) Ein neutronenbeugungsexperiment: A neutron diffraction experiment Helv. Phys. Acta 10 400

A lot of the early work was done here….

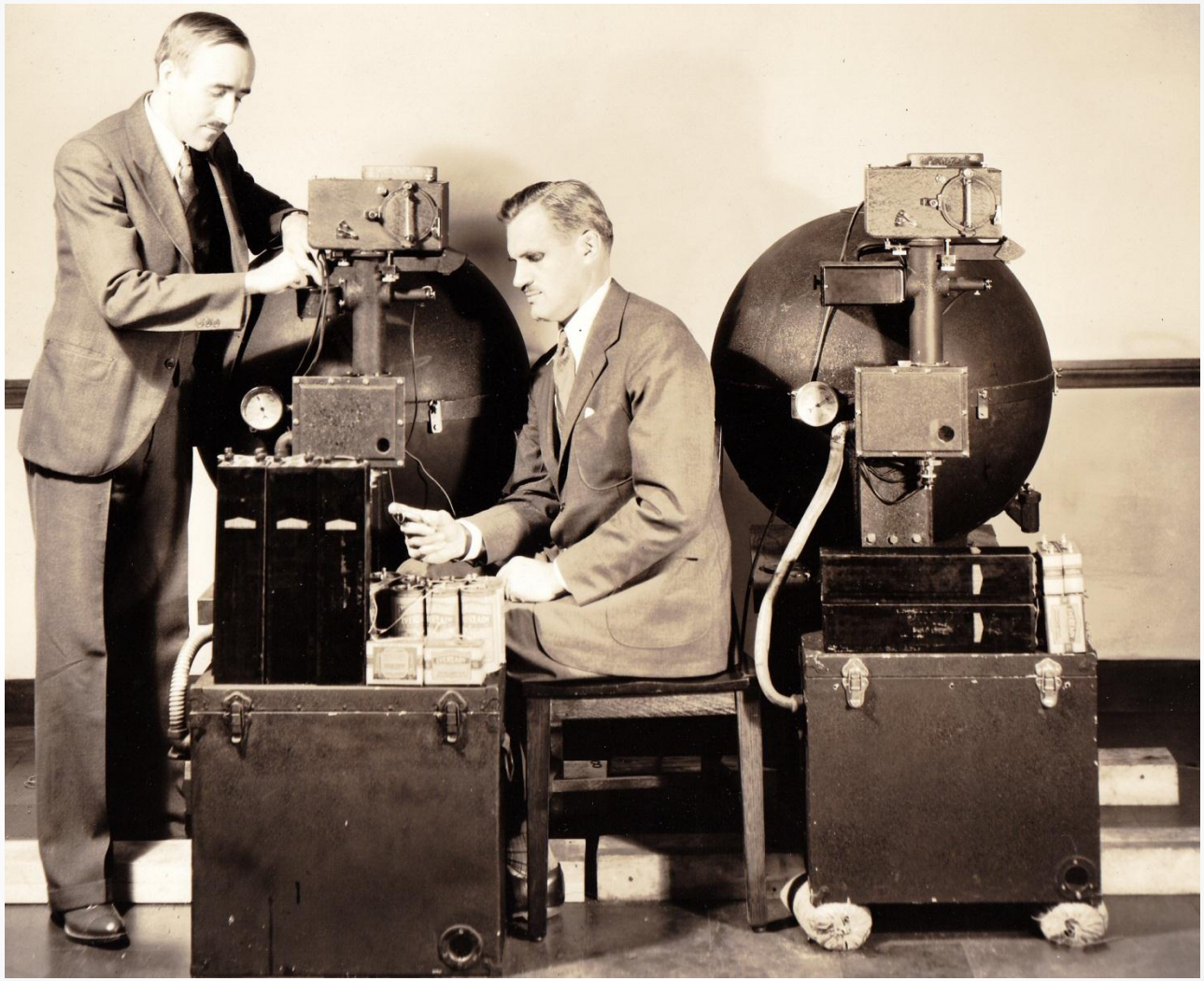
ORNL in 1943

The Clinton Pile was the world's first continuously operated nuclear reactor



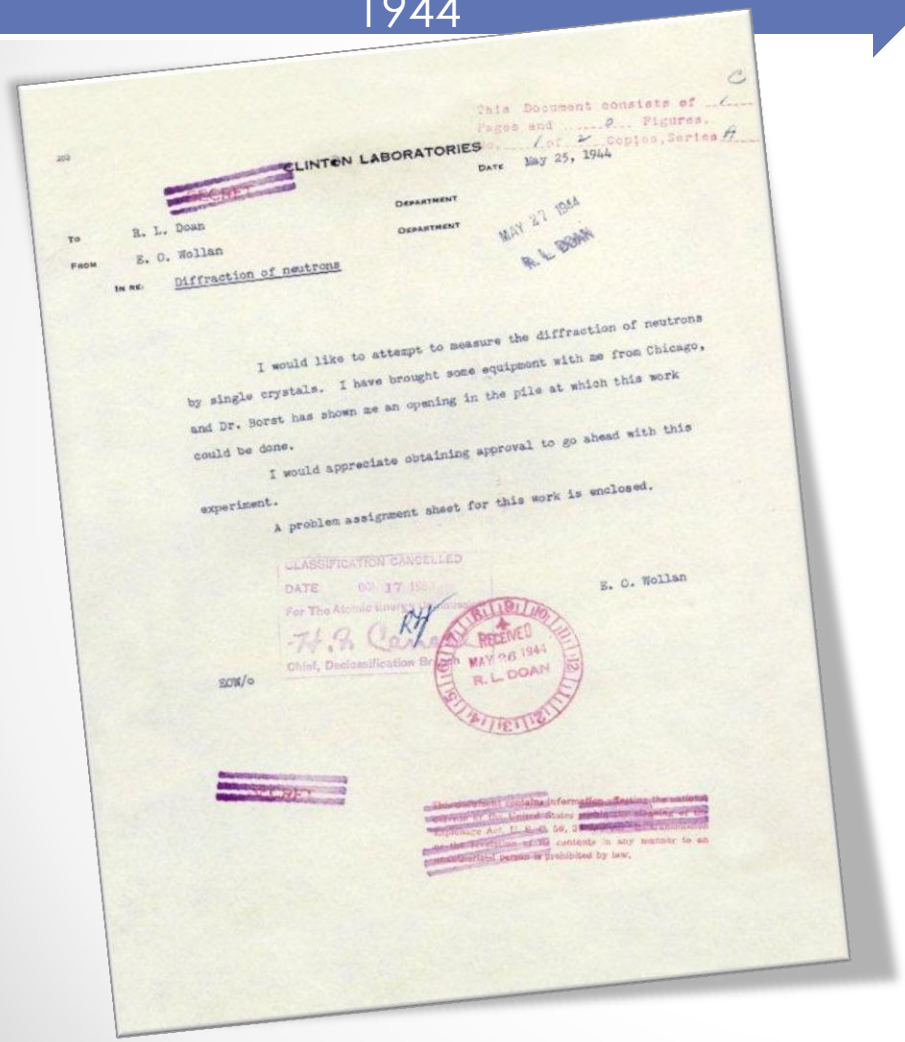
Managed by UT-Battelle
for the U.S. Department of Energy

Ernie O. Wollan (1902–1984)



The Nobel Prize proposal

1944 → 1994



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CLINTON LABORATORIES

Date May 25, 1944

Department

Department

To R. L. Doan

From E. O. Wollan

In re: Diffraction of neutrons

MAY 27 1944
R. L. DOAN

I would like to attempt to measure the diffraction of neutrons by single crystals. I have brought some equipment with me from Chicago, and Dr. Borst has shown me an opening in the pile at which this work could be done.

I would appreciate obtaining approval to go ahead with this experiment.

A problem assignment sheet for this work is enclosed.

E. O. Wollan

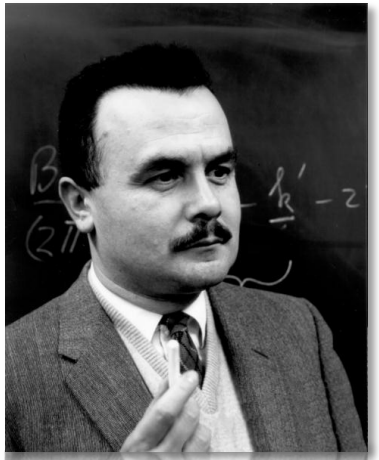
EOW/o

CLASSIFICATION CANCELLED
DATE OCT 17 1961
For The Atomic Energy Commission
Chief, Declassification Branch

RECEIVED
MAY 26 1944
R. L. DOAN

Awarded for "pioneering contributions to the development of neutron scattering techniques for studies of condensed matter"

Bertram N. Brockhouse



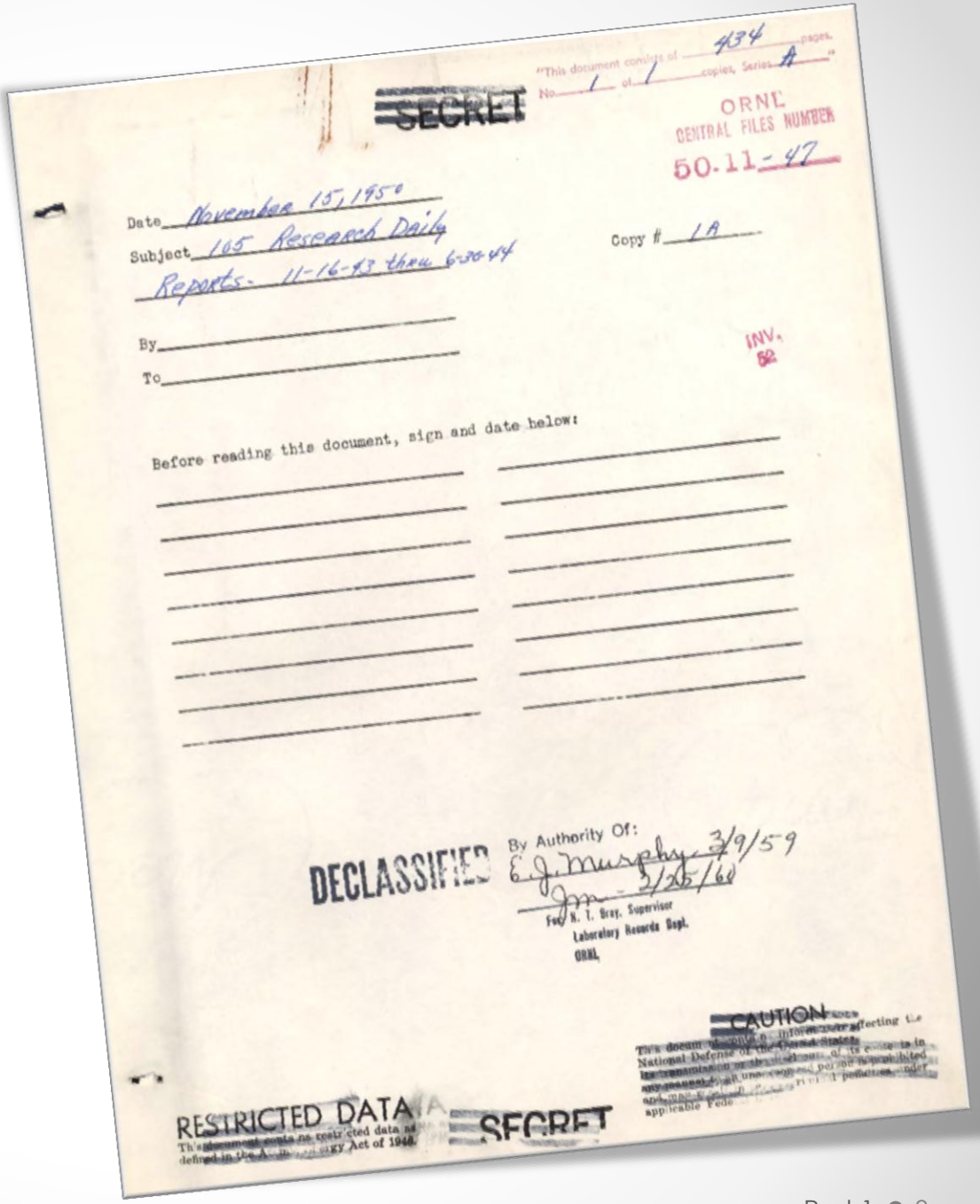
Development of neutron spectroscopy

Clifford G. Shull

Development of the neutron diffraction technique

Graphite Reactor

Pile Research Logs
Volume 1
November 1943–June 1944
Declassified in1960



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Laboratory Records Dept.
ORNL

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26 May 1944

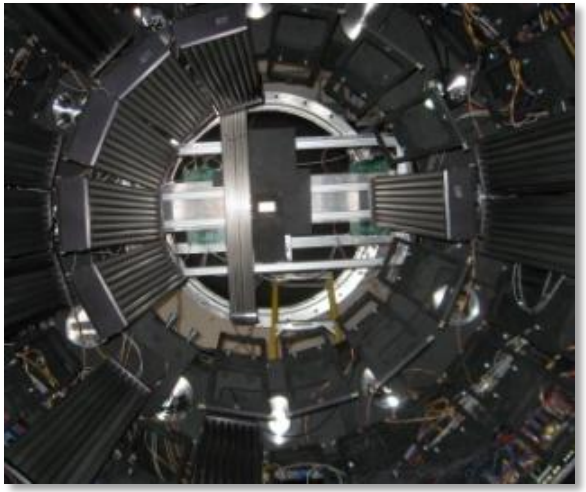
105 Research - Daily Report, May 26, 1944

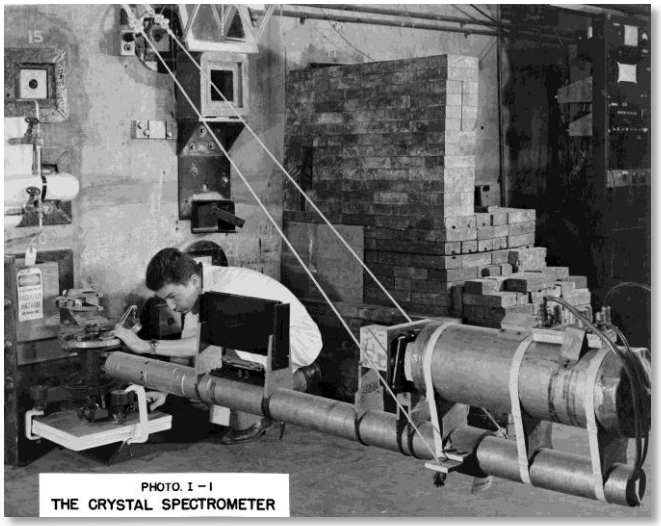
Neutron diffraction. The two south sections of the stringer in hole 52 (which is a foil slot) were replaced by two ordinary foil slot sections in order to give a channel ½" x 2" from the center of the pile to the surface of the shield. A neutron spectrometer consisting of a gypsum crystal 5/8" x 4" x 7" supported on a circle and capable of being rotated was placed in this beam. A cadmium shielded BF_3 counter, placed to receive the reflected radiation, showed a low background without the crystal. With the crystal in place, a satisfactory intensity was obtained which varied with the weight of the crystal. The maximum expected when the angle of incidence equalled the angle of reflection was not observed. This is probably due to the large energy distribution in the beam so that random scattering masked the effect desired. Experiments will be interrupted until a more satisfactory geometry has been constructed.

B Rabbit tunnels. The biologists exposed mice in the rabbit tunnels.

… poor mice!

And the instrumentation….





Some basics

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)

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

For L in meters, t in seconds, v in m/s, E in meV, and λ in Å

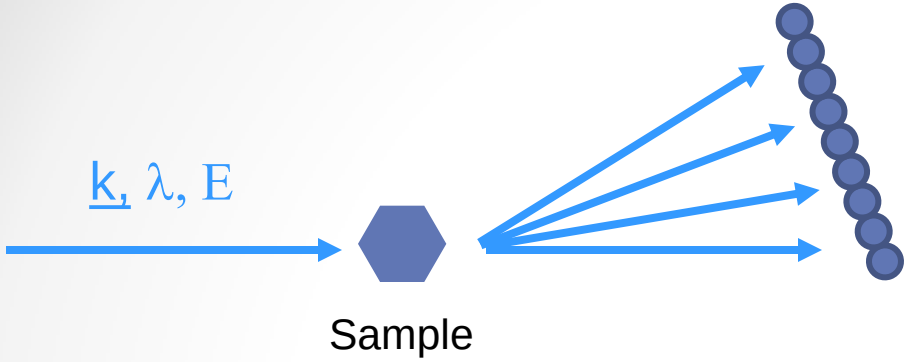
$E = 5.23 \times 10^{-6}\ v^2 = 81.8/\lambda^2$ $\qquad$ $\lambda = 3956/v = 3956\ t/L$

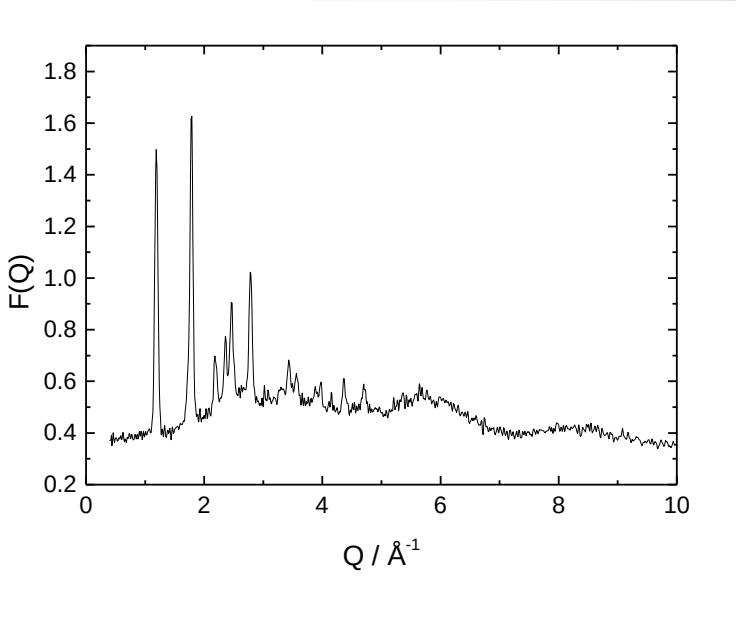
Room temperature ~ 25 meV ~ 0.18 nm ~ 2200 m/s

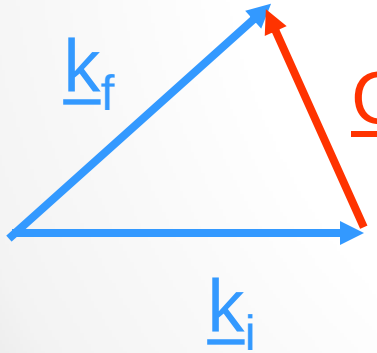
Brightness and fluxes for neutron and X-ray sources

	Brightness (s^{-1} m^{-2} $ster^{-1}$)	*dE/E* (%)	*Divergence* ($mrad^2$)	*Flux* (s^{-1} m^{-2})
Neutrons	10^{15}	2	10 x 10	10^{11}
Rotating Anode	10^{16}	3	0.5 x 10	5×10^{10}
Bending Magnet	10^{24}	0.01	0.1 x 5	5×10^{17}
Wiggler	10^{26}	0.01	0.1 x 1	10^{19}
Undulator (APS)	10^{33}	0.01	0.01 x 0.1	10^{24}

What do we measure?



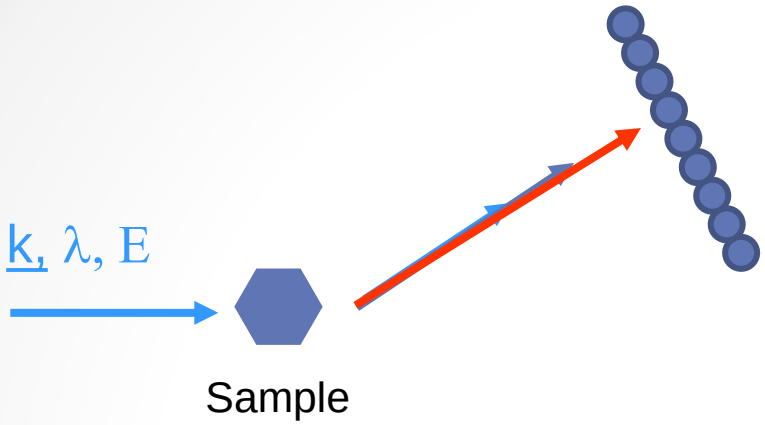


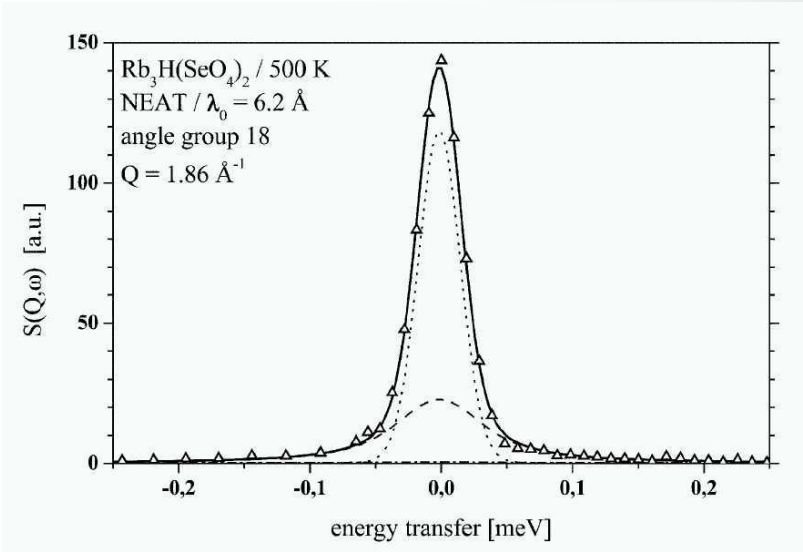


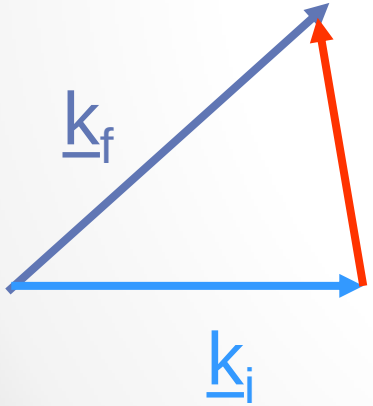
$\underline{Q} = \underline{k}_f - \underline{k}_i$ Wavevector transfer

$|k_f| = |k_i|$ "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 and we get?

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

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

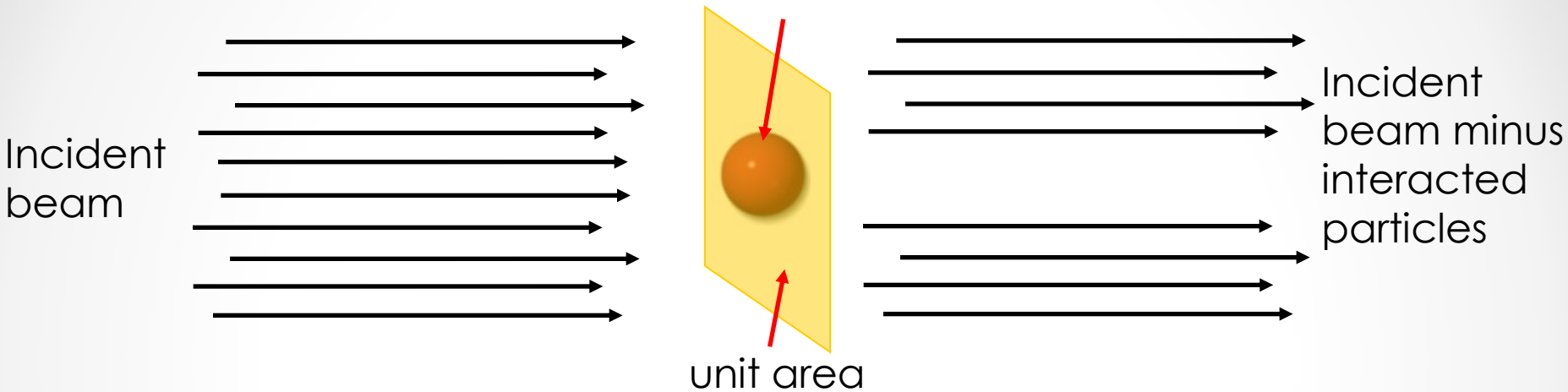
$$S_i(\vec{Q},\omega) = \frac{1}{h} \iint G_s(\vec{r},t) e^{i(\vec{Q}.\vec{r}-\omega t)} d\vec{r} dt$$

Inelastic coherent scattering measures correlated motions of atoms

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

Interaction cross-sections

Effective cross-sectional area of atom for event of type *i*



The interaction cross-section σ_i has units of area and is related to the probability of the event of type *i*

$$\sigma_i = \frac{\text{number of events}_i}{\text{number of incident particles / unit area}}$$

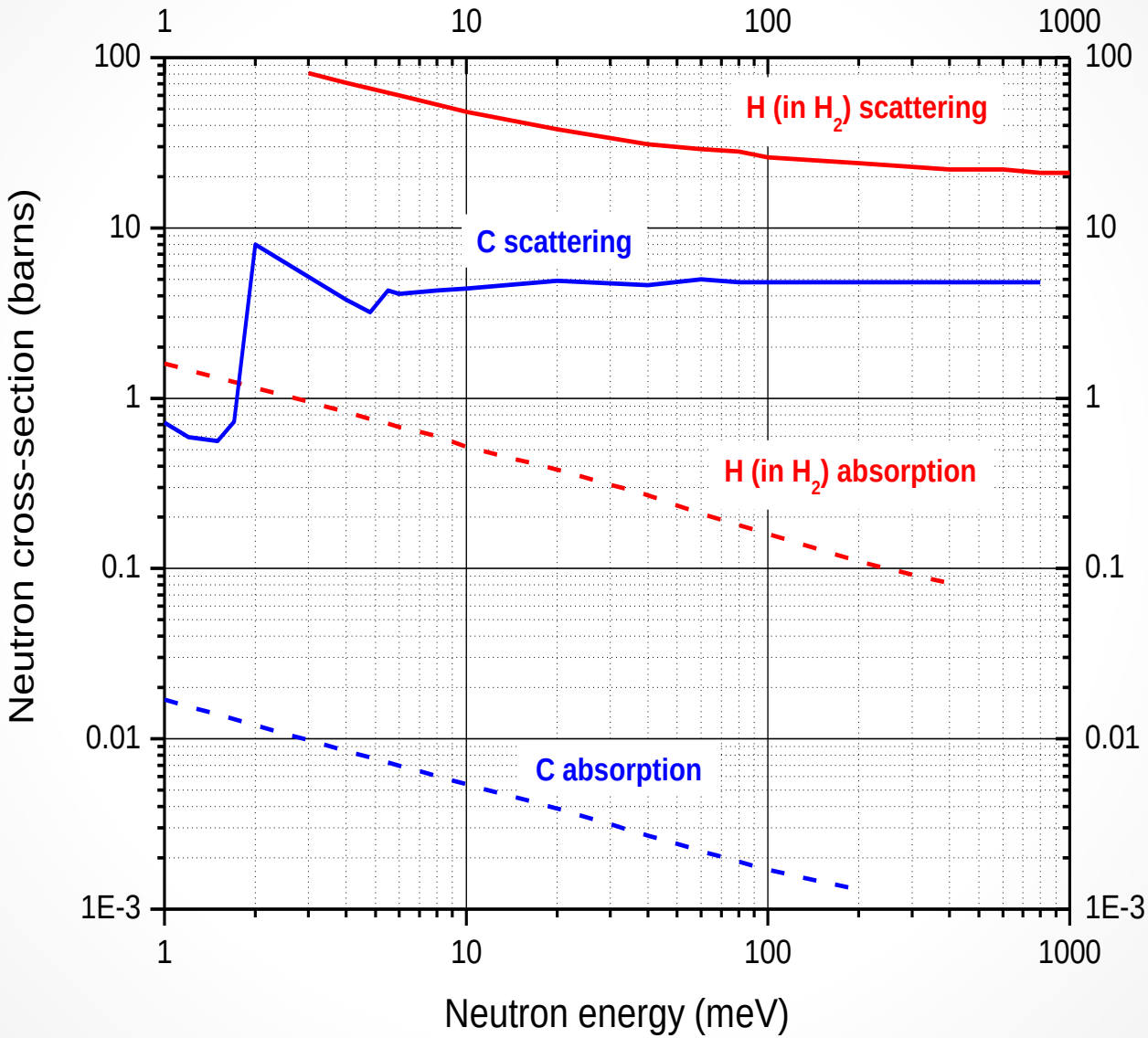
Units: 1 barn = 10^{-24} cm^2

Transmission = $e^{-N\sigma x}$

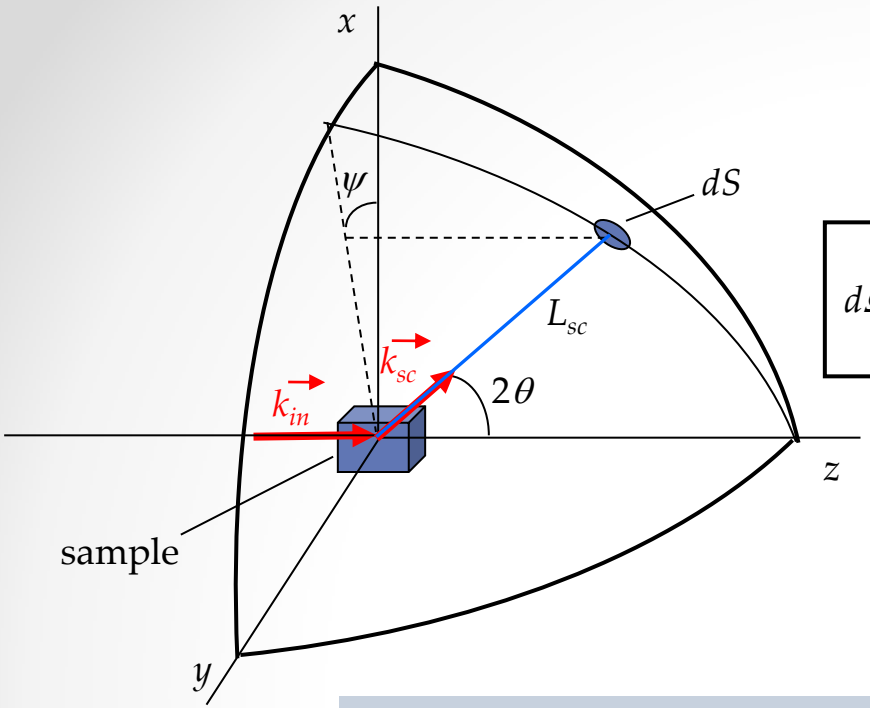
N = # of atoms per unit volume

x = thickness

Typical neutron cross-sections



Differential scattering cross-sections



$$d\Omega = \frac{dS}{L_{sc}^{\ 2}}$$

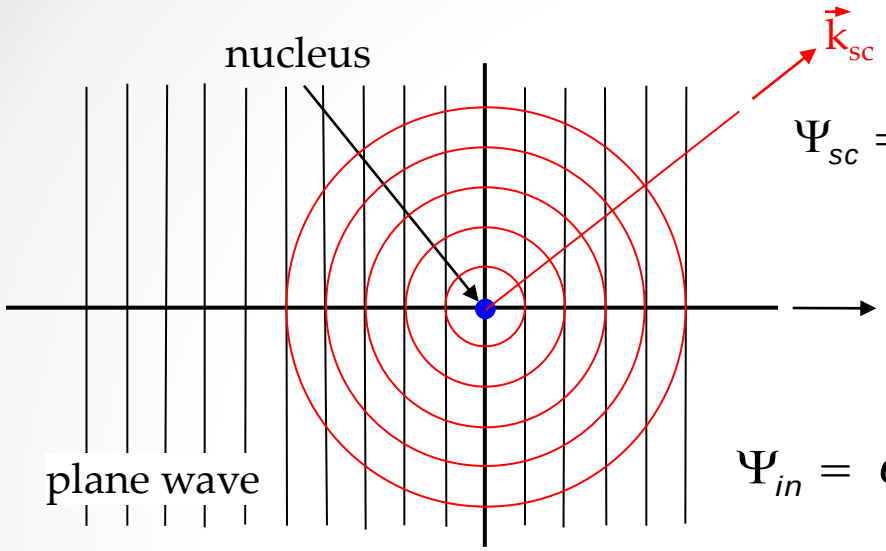
Φ = number of incident neutrons per cm^2 per second

$$\sigma = \frac{\text{total number of neutrons scattered per cm}^2\text{ per second}}{\Phi}$$

$$\frac{d\sigma}{d\Omega} = \frac{\text{number of neutrons scattered per cm}^2\text{ per second into } d\Omega}{\Phi\, d\Omega}$$

$$\frac{d^2\sigma}{d\Omega\, dE} = \frac{\text{number of neutrons scattered per cm}^2\text{ per second into } d\Omega \text{ and } dE}{\Phi\, d\Omega\, dE}$$

Neutron scattering from a stationary atom



$$\Psi_{sc} = \frac{-b}{R} e^{i\vec{k}_{sc}\cdot\vec{R}}$$

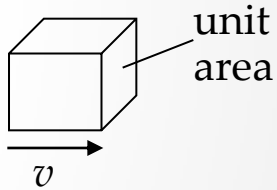
$$\Psi_{in} = e^{i\vec{k}_{in}\cdot\vec{R}}$$

$|\Psi|^2$ is the probability of finding a neutron per unit volume

$$|\Psi_{in}|^2 = 1$$

$$|\Psi_{sc}|^2 = b^2/R^2$$

$v\,|\Psi|^2$ is the number of neutrons crossing a unit area per unit time

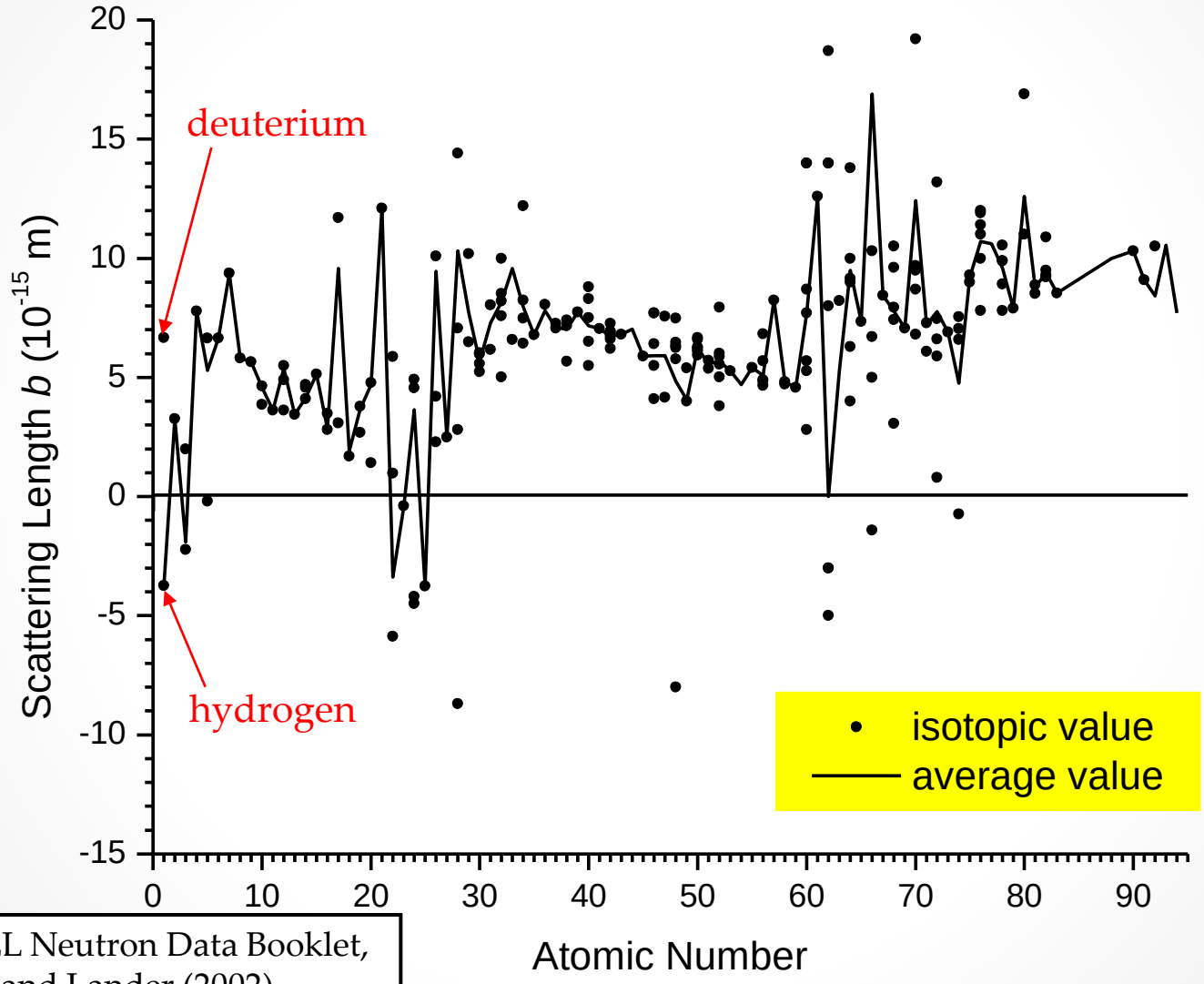


$$\left(\frac{d\sigma}{d\Omega}\right)_0 = \frac{\text{number scattered per unit solid angle per unit time}}{\text{number incident per unit area per unit time}} = \frac{vb^2}{v} = b^2$$

$$\sigma_{tot\text{-}scat} = 4\pi b^2$$

b is the "neutron scattering length" of the atom

Neutron scattering lengths vary with element and isotope



Data from ILL Neutron Data Booklet, ed. Dianoux and Lander (2002)

The measurement process

What do we measure for elastic scattering?

We want to know the **differential scattering cross-section (scattering probability)** ($d\sigma/d\Omega$) for elastic scattering, or ($d^2\sigma/d\Omega dE$) for inelastic scattering

For **elastic** scattering, the relevant quantity is ($d\sigma/d\Omega$), which is a function of $\vec{Q}$ and is the probability a neutron with wavelength λ will be scattered into the solid angle $d\Omega$ centered about the nominal scattering angle 2θ and the azimuthal angle ψ

[Note that λ, 2θ, and ψ together are sufficient to define $\vec{Q}$]

To determine $\vec{Q}$, we need to determine **one** wavelength and the position of the detected event relative to the sample and the incident beam

What do we measure, elastic – cont'd?

To measure ($d\sigma/d\Omega$), we measure the **counts [detected neutrons]** per unit time $C(\lambda,2\theta,\psi)$ in a detector covering a solid angle $\Delta\Omega$ at a scattering angle 2θ and azimuthal angle ψ at a wavelength λ

To express this as a probability, divide by the number of incident neutrons per unit area per unit time $\Phi(\lambda)$ **[incident spectrum]**

Some of the counts in the detector will be due to background - not to scattering from the sample. The **background** $B(\lambda,2\theta,\psi)$ must be measured and subtracted to get the true sample scattering

$$\frac{d\sigma}{d\Omega}(\lambda,2\theta,\psi) \approx \frac{C(\lambda,2\theta,\psi)-B(\lambda,2\theta,\psi)}{N\Phi(\lambda)\Delta\Omega}$$

N is the number of scattering atoms in the sample (single atom type)

What do we measure for inelastic scattering?

For **inelastic** scattering, the relevant quantity is ($d^2\sigma/d\Omega dE$), which is a function of $\vec{Q}$ and E and is the probability a neutron with wavelength λ_{in} will be scattered into the solid angle $d\Omega$ centered at the nominal scattering angle 2θ and the azimuthal angle ψ, and will change its wavelength to $\lambda_{sc} \neq \lambda_{in}$

[Note that λ_{in}, λ_{sc}, 2θ, and ψ are sufficient to define $\vec{Q}$ and E]

We need to determine **<u>two</u>** wavelengths and the position of the detected event relative to the sample and the incident beam

What do we measure, inelastic – cont'd?

To measure ($d^2\sigma/d\Omega dE$), we measure the **counts [detected neutrons]** per unit time $C(\lambda_{in},\lambda_{sc},2\theta,\psi)$ in a detector covering a solid angle $\Delta\Omega$ around a scattering angle 2θ and azimuthal angle ψ at incident and scattered wavelengths λ_{in}, λ_{sc} consistent with a range ΔE of energy transfers.

To express this as a probability, divide by the number of incident neutrons per unit area per unit time $\Phi(\lambda_{in})$ **[incident spectrum]** .

Here also, the **background** $B(\lambda_{in},\lambda_{sc},2\theta,\psi)$ must be measured and subtracted to get the true sample scattering.

$$\frac{d^2\sigma}{d\Omega dE}(\lambda_{in},\lambda_{sc},2\theta,\psi) \approx \frac{C(\lambda_{in},\lambda_{sc},2\theta,\psi)-B(\lambda_{in},\lambda_{sc},2\theta,\psi)}{N\Phi(\lambda_{in})\Delta\Omega\Delta E}$$

N is the number of scattering atoms in the sample (single atom type)

Determining the elastic or inelastic scattering probability: basic needs

We need a source of neutrons with wavelengths in the right range

We need to determine incident and scattered neutron directions [**collimation**]

→ Collimation determines the uncertainty $\delta(2\theta)$ in the scattering angle [**angular resolution**]

We need to determine one wavelength (elastic) or two wavelengths (inelastic). This can be done by :

→ Bragg diffraction (crystal monochromator)

→ Time-of-flight

Either of these methods leads to uncertainties $\delta\lambda_{in}$, $\delta\lambda_{sc}$ in the incident and scattered wavelengths [**wavelength resolution**]

Determining the scattering probability

We need detectors to measure the counts at different scattering angles

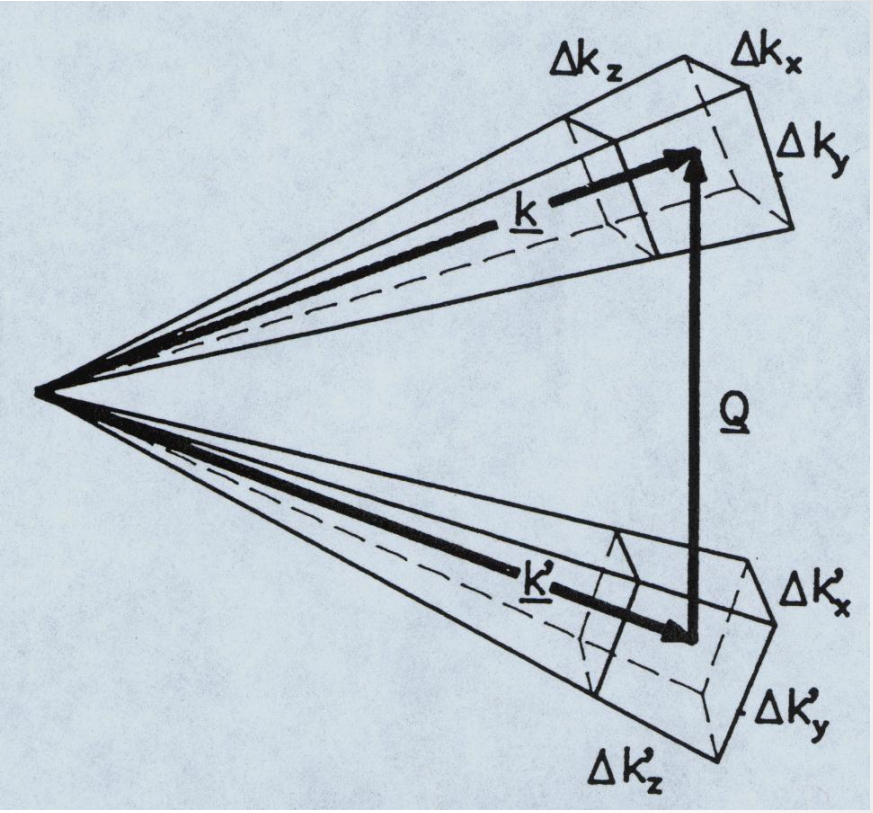
In order to cover the desired range, we need to make measurements at many wavelengths and/or many scattering angles [*Q*-range, *E*-range]

To properly normalize the data, we need to determine the number of incident neutrons per unit area per unit time $\Phi(\lambda)$ at each wavelength

Instrumental Resolution

- Uncertainties in the neutron wavelength and direction of travel imply that Q and E can only be defined with a certain precision

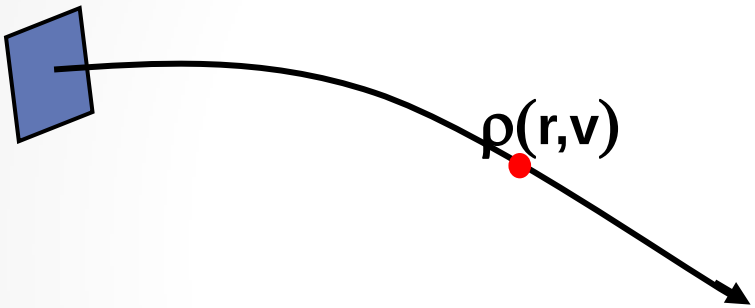
- The total signal in a scattering experiment is proportional to the phase space volume within the elliptical resolution volume – the better the resolution, the lower the count rate



More on resolution in Roger Pynn's lecture

Resolution versus Intensity?

Liouville theorem:
Phase space density ρ is constant along particle trajectories of any length in conservative force fields



No. of particles hitting in unit time a surface df perpendicular to trajectory (local z axis):

$N = \rho\, dx\, dy\, dz\, dv_x dv_y dv_z =$

$= \rho\, dx\, dy\, v\, v\alpha_x\, v\alpha_y\, v^2 d\lambda\, m/h \propto$

$\propto \phi(\lambda)\, df\, d\Omega\, d\lambda$

where:

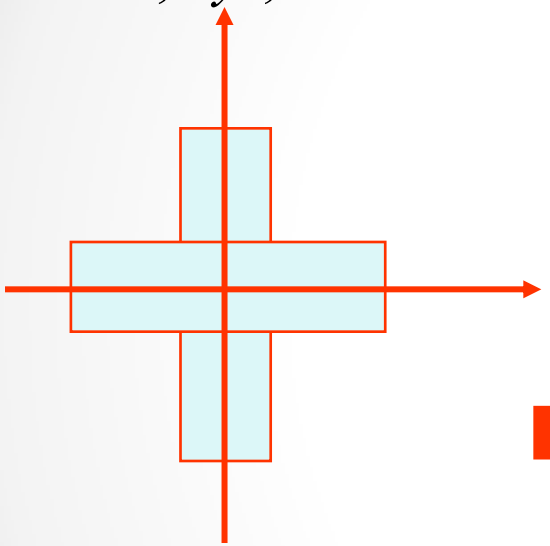
$d\Omega$ = beam divergence solid angle

$d\lambda$ = neutron wavelength spread

Compromise between resolution (δv, $\delta\Omega$) and intensity:
Avoid using better resolution than absolutely needed in each individual case!

Liouville's Theorem: a practical definition

Beam divergence
$\Delta x', \Delta y', \Delta z'$



The beam emittance $\Delta x.\Delta x'$ is constant

Beam size
$\Delta x, \Delta y, \Delta z$

Focussing : Size ↘ and divergence ↗

Collimating : Size ↗ and divergence ↘

The phase space density of neutrons cannot be increased (no collisions)
Due to absorption and finite efficiency of optical elements,
the phase space density decreases

Some typical components of Neutron Scattering Instruments

Monochromators	Monochromate or analyze the energy of a neutron beam
Collimators	Define the direction of travel of the neutron
Guides	Allow neutrons to travel large distances without suffering intensity loss
Choppers	Define a short pulse or pick out a small band of neutron energies
Detectors	Detect neutrons – can be position sensitive, and time coded
Polarizers	Select an orientation of a the neutron spin
Spin turn coils	Manipulate the neutron spin using Larmor precession
Shielding	Minimize background and radiation exposure to users and detectors

What we will cover in Part 2

- Simple collimation devices
- Reflection devices
- Beam transport in neutron guides
- Introduction to supermirrors

Summary

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Reading material

- ILL Neutron Data Booklet (2002):
  - http://neutrons.ornl.gov/why/NeutronDataBooklet.pdf
- Neutron Scattering: A Primer by Roger Pynn (1990):
  - http://library.lanl.gov/cgi-bin/getfile?19-01.pdf
  - http://la-science.lanl.gov/cat_materials.shtml#neutron
- International Tables of Crystallography Vol. C (2004)
  - http://www.springerlink.com/content/q81j2r10u517qxq3/

Thank you!