Neutron Sources

PART 1

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European Spallation Source

Acknowledgment

This lecture relies on the precious input and materials from:

ESS: Axel Steuwer, Mats Lindroos, Colin Carlite, Ferenc Mezei, Konstantin Batkov, Luca Zanini

EPFL: Giorgio Margaritondo

INFN/ESS: Santo Gammino

CNRS/ESS: Sebastien Bousson and Alex Mueller

A special thanks to Mats Lindroos, who donated the money received for his 50th birthday to invite few students to this school.

Outline

PART 1
- Background for neutron course
- Neutrons properties and their interactions
- Applications using Neutrons

PART 2
- How to generate intense neutron beams
- High power proton linear accelerator

PART 3
- Examples of world-wide neutron sources

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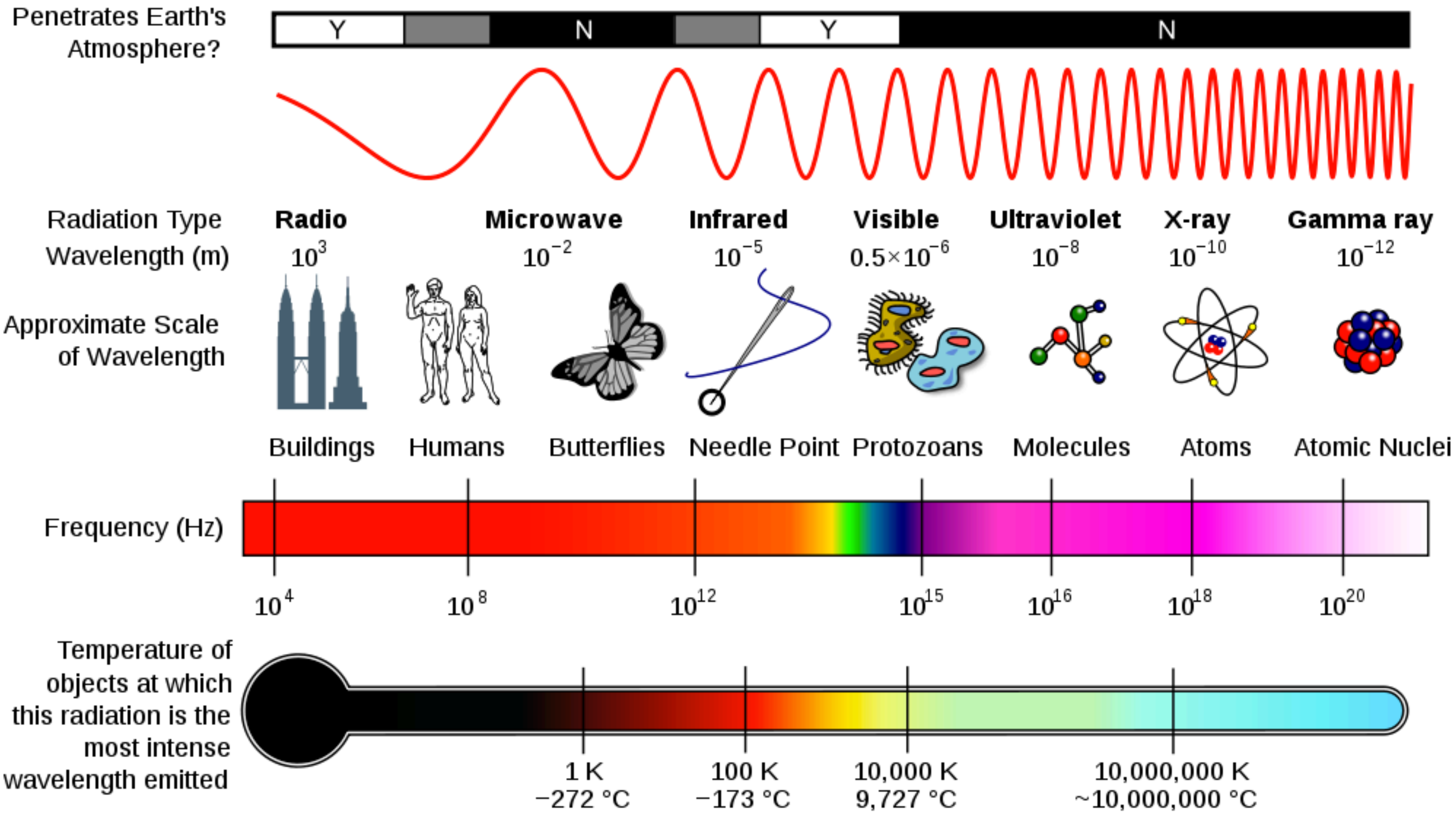
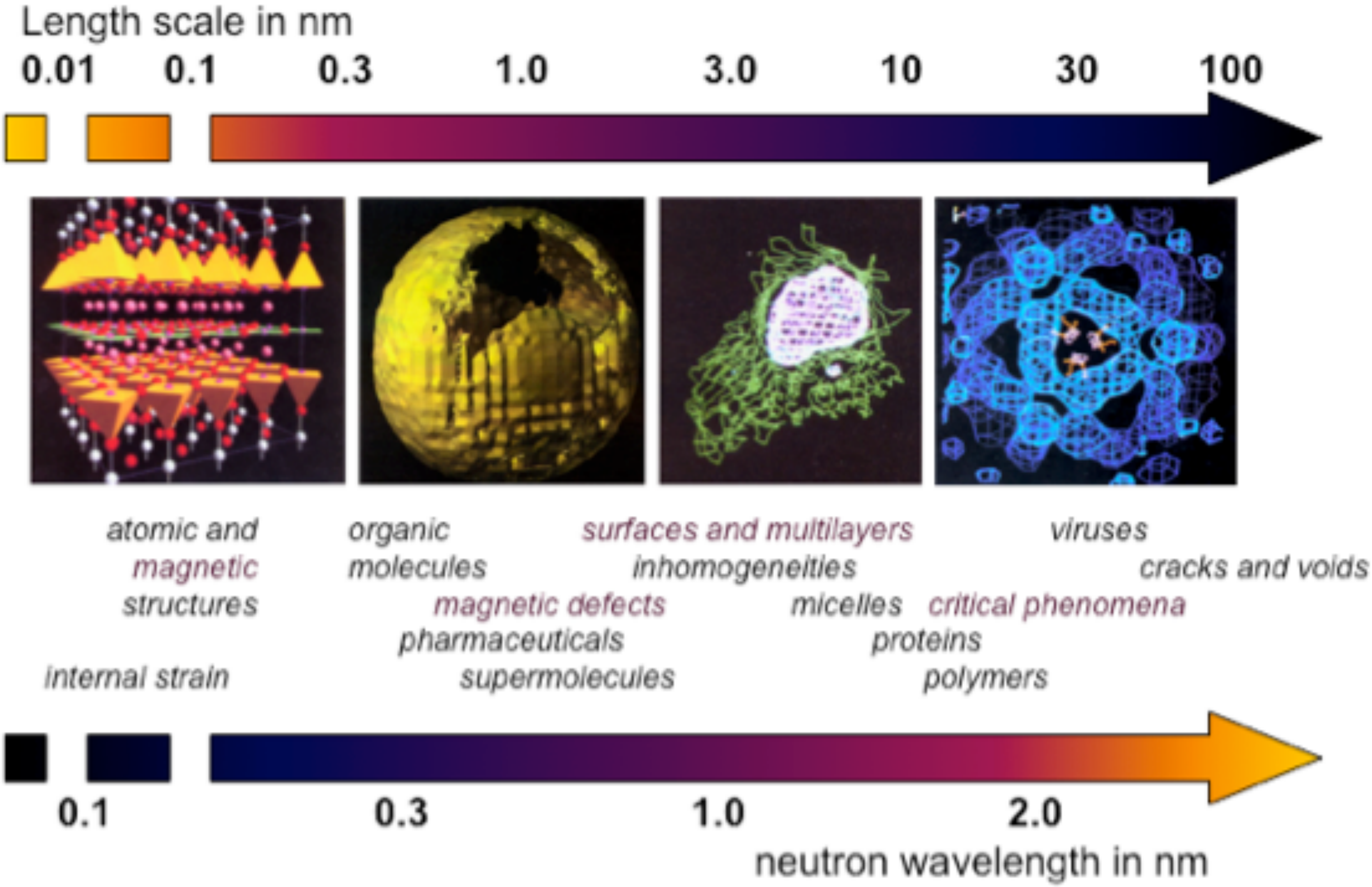
Context – Reference to ASP2012 Classes:

- Ketevi Assamagan: Nuclear Physics (July 16 and 18)
- Lenny Rivkin: Particle beam dynamics, beam optics, instrumentations and light sources
- Lyn Evans: Accelerator sciences and the LHC
- Herman Winick: Light Sources

Electro-magnetic Spectrum



Neutron Microscope – Length scales



Length scale in nm

0.01 0.1 0.3 1.0 3.0 10 30 100

atomic and
magnetic
structures

organic
molecules

surfaces and multilayers

inhomogeneities

viruses

cracks and voids

magnetic defects

micelles

critical phenomena

pharmaceuticals

proteins

internal strain

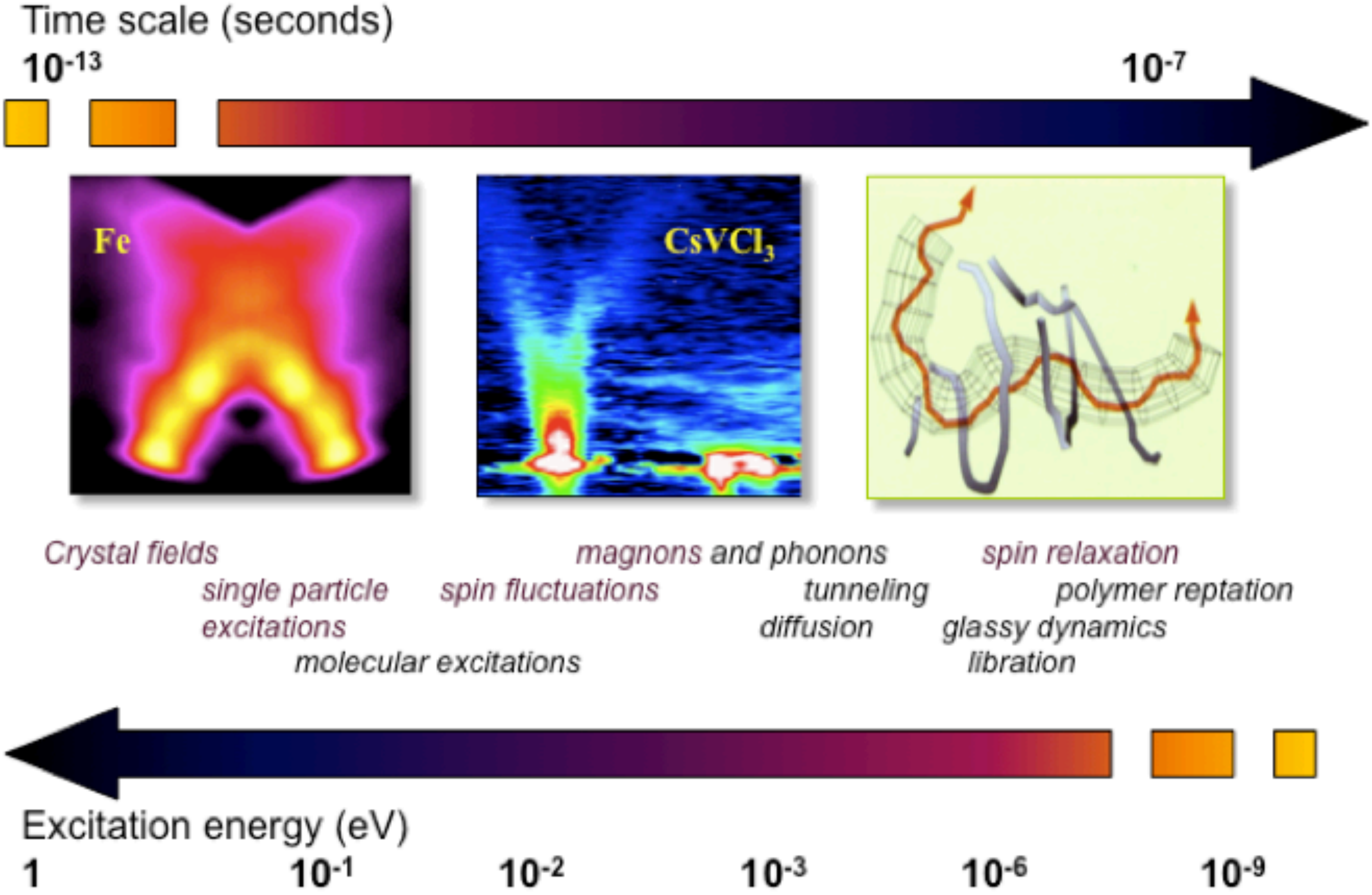
supermolecules

polymers

0.1 0.3 1.0 2.0

neutron wavelength in nm

Neutron Microscope – Time and energy scales



Time scale (seconds)

10^{-13} 10^{-7}

Crystal fields

single particle excitations

molecular excitations

spin fluctuations

magnons and phonons

tunneling

diffusion

spin relaxation

polymer reptation

glassy dynamics

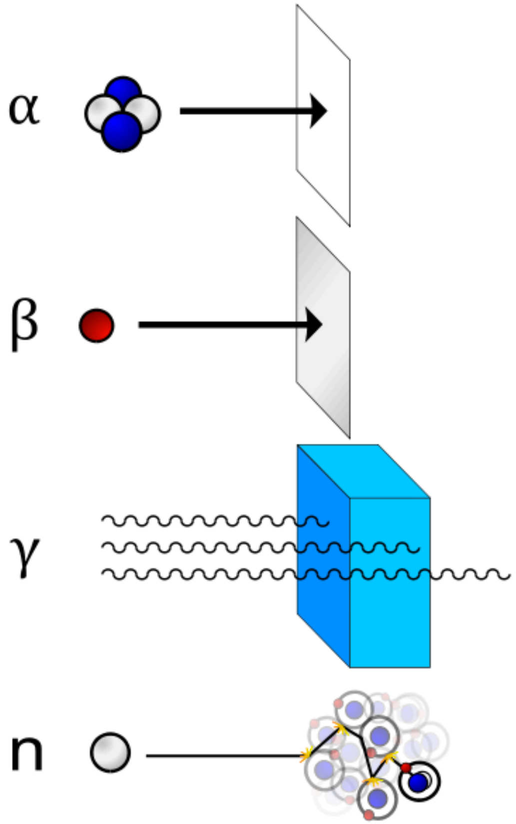
libration

Excitation energy (eV)

1 10^{-1} 10^{-2} 10^{-3} 10^{-6} 10^{-9}

Ionizing Radiation

Ionizing radiation is radiation composed of particles that individually carry enough energy to liberate an electron from an atom or molecule without raising the bulk material to ionization temperature.



When ionizing radiation is emitted by or absorbed by an atom, it can liberate a particle.
Such an event can alter chemical bonds and produce ions, usually in ion-pairs, that are especially chemically reactive.

Note: Neutrons, having zero electrical charge, do not interact electromagnetically with electrons, and so they cannot *directly* cause ionization by this mechanism.

➔ High precision non-destructive probe … why ?

Discovery of the Neutron

1920 **E. Rutherford**: disparity between the atomic number of an atom and its atomic mass could be explained by a neutral particle within atomic nucleus.

1930 **V. Ambartsumian and D. Ivanenko**: proved that the nucleus cannot consist of protons and electrons only.

1931 **W. Bothe and H. Becker**: interactions of α-particles with light nuclei (Li, Be, B) produce an unusually penetrating radiation.

1932 **Irène Joliot-Curie and F. Joliot**: interactions of *beryllium radiation* with hydrogen-containing compounds ejects energetic protons (moderation).

80th Birthday – June 1st, 2012

--------- Original Message ---------

Subject: The neutron's 80th birthday

Date: Fri, 01 Jun 2012 12:29:01 +0200

From: Francoise Vauquois <vauquois@ill.fr>

To: gen_l@ill.fr

Dear all,

It is 80 years today since the publication by the Royal Society of Cambridge Physicist James Chadwick's famous paper proving the existence of the neutron - on 1 June 1932. Chadwick was awarded the Nobel Prize for his paper two years later.

Chadwick's discovery launched the development of neutron research, which has since made incontestably decisive break-throughs for modern science. And the ILL has been world-leading in this domain! 2012 is also the fortieth anniversary of the start of experiments with neutrons at ILL, in 1972.

You will find more on the history of Chadwick's discovery on the ILL website:
http://www.ill.eu/fr/news-events/presse/communiques-de-presse/lill-fete-les-80-ans-du-neutron-1062012/

You can also hear the ILL director, Andrew Harrison, interviewed for the occasion by the BBC, by visiting the BBC's site, on
http://www.bbc.co.uk/programmes/b01j6t0n

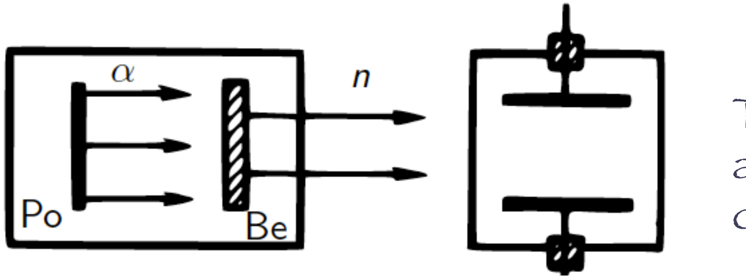
The French newspaper Le Figaro has also marked the occasion:
http://www.lefigaro.fr/sciences/2012/05/24/01008-20120524ARTFIG00844-le-neutron-fete-ses-80-ans-cette-annee.php

and so did Spain's Muy interesante:
http://www.muyinteresante.es/el-neutron-cumple-80-anos?utm_source=twitter&utm_medium=socialoomph&utm_campaign=muy-interesante-twitter689

James Chadwick 1932 (α,n) reaction

$${}^{4}_{2}He + {}^{9}_{4}Be \rightarrow {}^{12}_{6}C + {}^{1}_{0}n$$

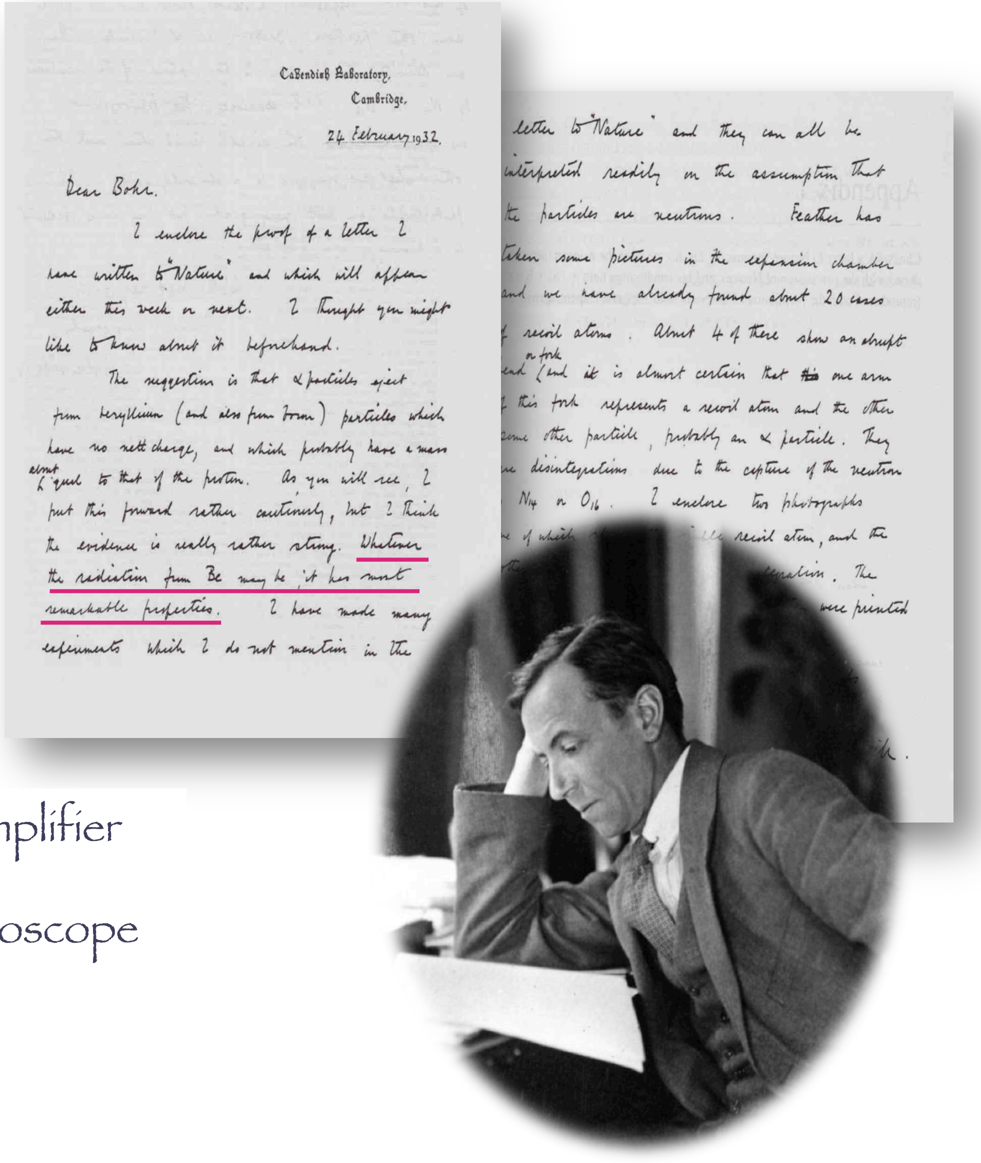
"Whatever the radiation from Be may be, it has most remarkable properties"



To amplifier
and
oscilloscope

Neutron chamber

Ionization chamber



Cavendish Laboratory,
Cambridge,
24 February 1932.

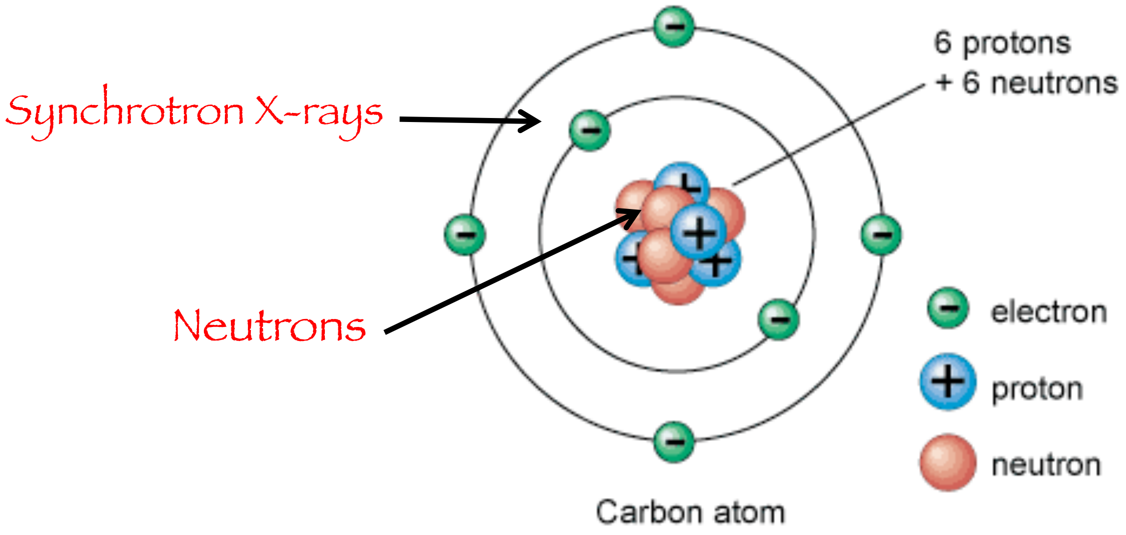
Dear Bohr.

I enclose the proof of a letter I have written to "Nature" and which will appear either this week or next. I thought you might like to know about it beforehand.

The suggestion is that α particles eject from beryllium (and also from boron) particles which have no nett charge, and which probably have a mass about equal to that of the proton. As you will see, I put this forward rather cautiously, but I think the evidence is really rather strong. Whatever the radiation from Be may be, it has most remarkable properties. I have made many experiments which I do not mention in the

letter to "Nature" and they can all be
interpreted readily on the assumption that
the particles are neutrons. Feather has
taken some pictures in the expansion chamber
and we have already found about 20 cases
f recoil atoms. About 4 of these show an abrupt
end or fork (and it is almost certain that ~~the~~ one arm
f this fork represents a recoil atom and the other
some other particle, probably an α particle. They
e disintegrations due to the capture of the neutron
N_{14} or O_{16}. I enclose two photographs
e of which [illegible] recoil atom, and the
[illegible] The
[illegible] were printed

Neutrons Properties



Note: X-rays are emitted by electrons outside the nucleus, while gamma rays are emitted by the nucleus.

1.675×10^{-27} kg Mass	939.57 MeV	$m_n \approx m_p + 2.5 m_e$
Mean lifetime	15 min	$n \longrightarrow p + e^- + \bar{\nu}_e$
Composition	udd	hadron
Electric charge	0	high penetration
Magnetic moment	$-1.04\,\mu_B$	feels the nucleus

Neutron Energy

$$E = k_B T$$

$$E = k_B T = \tfrac{1}{2} m v^2 = \frac{h}{2m\lambda^2}$$

$$\lambda = \frac{h}{mv}$$

Boltzmann distribution

De Broglie

$$E\,[meV] = 0.0862\,T\,[K] = 5.22\,v^2\,[km/s] = 81.81\frac{1}{\lambda^2}\,[A]$$

Source	Energy	Temperature	Wavelength
cold	0.1-10	1-120	30-3
thermal	5-100	60-1000	4-1
hot	100-500	1000-6000	1-0.4

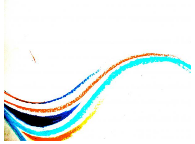
Why neutrons?

- Wavelengths comparable to interatomic spacings (1-5 Å)
- Energies comparable to structural and magnetic excitations (1-100 meV)
- Neutrons interact only weakly with matter
- Neutrons are deeply penetrating (bulk samples can be studied)
- Neutrons are scattered with a strength that varies randomly from element to element (and isotope to isotope) – tuning ?
- Neutrons have a magnetic moment : $\mu_n = -1.913\ \mu_N$

➔ *Neutron scattering is therefore an ideal probe of magnetic and atomic structures and excitations*

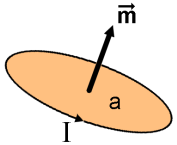
Why neutrons?

Wave



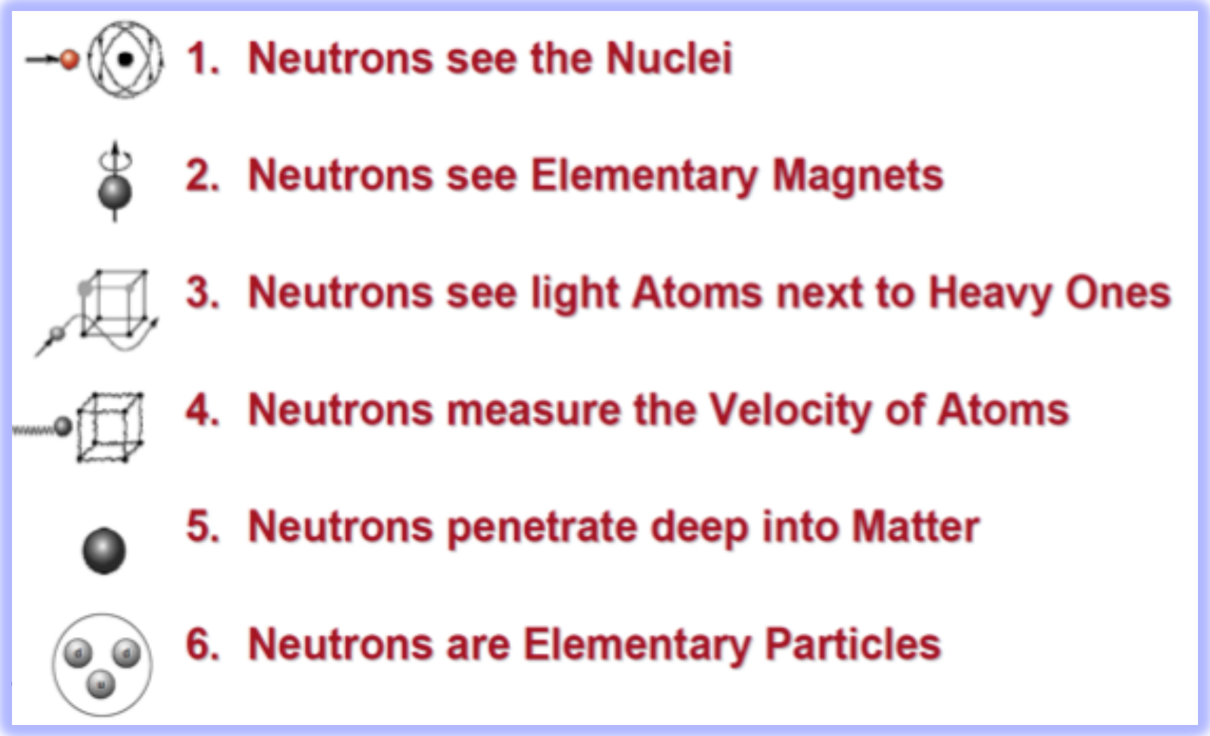
Particle

Magnetic moment



Neutral

Neutron properties are used to understand the nature of the solid and liquid states of matter, as an analytical tool to aid the development of materials and as a tool to examine curiosity-driven research that spans from cosmology, superconductivity to the dynamics of the molecules of life.



1. Neutrons see the Nuclei
2. Neutrons see Elementary Magnets
3. Neutrons see light Atoms next to Heavy Ones
4. Neutrons measure the Velocity of Atoms
5. Neutrons penetrate deep into Matter
6. Neutrons are Elementary Particles

Why neutrons? See http://www.ill.eu

Electrically Neutral – neutrons are non-destructive and can penetrate deep into matter. This makes them an ideal probe for biological materials and samples under extreme conditions of pressure, temperature, magnetic field or within chemical reaction vessels.

Microscopically Magnetic – they possess a magnetic dipole moment which makes them sensitive to magnetic fields generated by unpaired electrons in materials. Precise information on the magnetic behavior of materials at atomic level can be collected. In addition, the scattering power of a neutron off an atomic nucleus depends on the orientation of the neutron and the spin of the atomic nuclei in a sample. This makes the neutron a powerful instrument for detecting the nuclear spin order.

Ångstrom wavelengths – neutron wavelengths range from 0.1 Å to 1000 Å, making them an ideal probe of atomic and molecular structures, be they single atomic species or complex biopolymers.

Energies of millielectronvolts – their energies are of the same magnitude as the diffusive motion in solids and liquids, the coherent waves in single crystals (phonons and magnons), and the vibrational modes in molecules. It is easy to detect any exchange of energy between a sample of between 1microeV (even 1 neV with spin-echo) and 1eV and an incoming neutron.

Randomly sensitive – with neutrons the variation in scattering power from one nucleus to another within a sample varies in a quasi-random manner. This means that lighter atoms are visible despite the presence of heavier atoms, and neighboring atoms may be distinguished from each other. In addition, contrast can be varied in certain samples using isotopic substitution (for example D for H, or one nickel isotope for another); specific structural features can thus be highlighted. The neutron is particularly sensitive to hydrogen atoms; it is therefore a powerful probe of hydrogen storage materials, organic molecular materials, and biomolecular samples or polymers.

The Nobel Prize in Physics 1994

Neutrons behave as particles and as waves

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

Neutrons reveal structure and *dynamics*

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

Shull made use of **elastic scattering** i.e. of neutrons which change direction without losing energy when they collide with atoms.

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

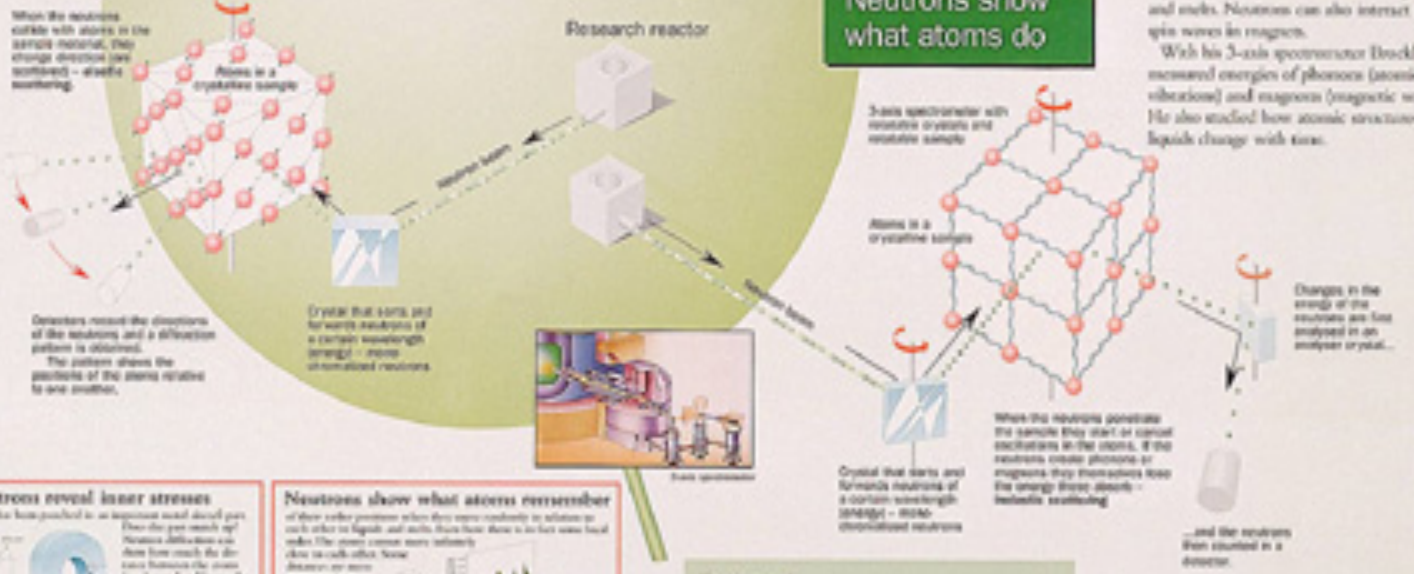
The pattern also shows how atomic dipoles are oriented in magnetic materials, since neutrons are affected by magnetic forces. Shull also made use of this phenomenon in his neutron diffraction technique.

[illegible]

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

Brockhouse made use of **inelastic scattering** i.e. of neutrons, which change both direction and energy when they collide with atoms. They then start or cancel atomic oscillations in crystals and record movements in liquids and melts. Neutrons can also interact with spin waves in magnets.

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



Neutrons show where atoms are

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

Neutrons show what atoms do

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) – monochromatised neutrons

3-axis spectrometer with rotatable crystals and rotatable sample

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

Crystal that sorts and forwards neutrons of a certain wavelength (energy) – mono-chromatised neutrons

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

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

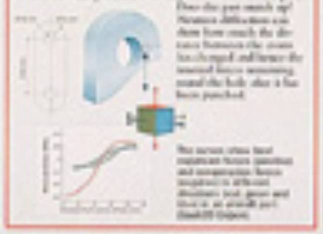
Neutrons see more than X-rays

X-rays are scattered by electrons, neutrons by atomic nuclei. With X-rays it is easiest to see atoms that have many electrons. Hydrogen, for example, which has only one electron, is not so easy to see. With neutrons, all kinds of atoms are visible.

[illegible]

Neutrons reveal inner stresses

A hole has been punched in an important metal aircraft part. Does the part match up? Neutron diffraction can show how much the distance between the atoms has changed and hence the internal forces remaining round the hole after it has been punched.



[illegible]

Neutrons show what atoms remember

of their earlier positions when they move randomly in relation to each other in liquids and melts. Even here there is in fact some local order. The atoms cannot move infinitely close to each other. Some distances are more common than others.

[illegible]

How it started

Brockhouse and Shull made their pioneering contributions at the first nuclear reactors in the USA and Canada back in the 1940s and 1950s. It was then that the neutrons of the reactor became available for peacetime research.

... how it continues

Thousands of researchers are now working at the many neutron research centres throughout the world. New and very advanced neutron scattering installations have been built and more are planned in Europe, the USA and Asia. At these super-installations the researchers are studying the structure of new ceramic superconductors, molecular monolayers on surfaces of catalytic exhaust cleaning, virus structures and the connection between the structure and the elastic properties of polymers.

KUNGL. VETENSKAPSAKADEMIEN
THE ROYAL SWEDISH ACADEMY OF SCIENCES

[illegible]

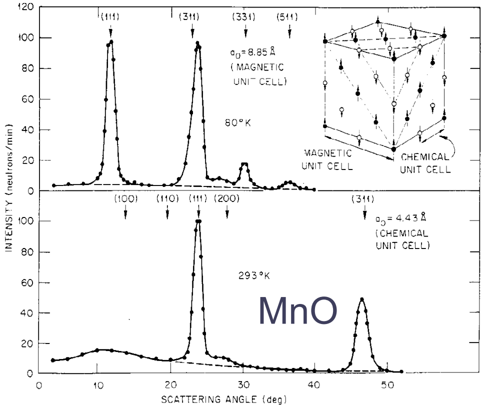
Further reading:

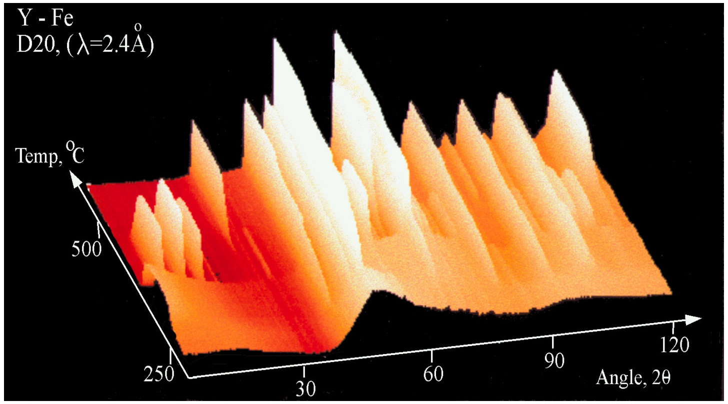
- [illegible]
- [illegible]
- [illegible]

Historic – Why neutrons?

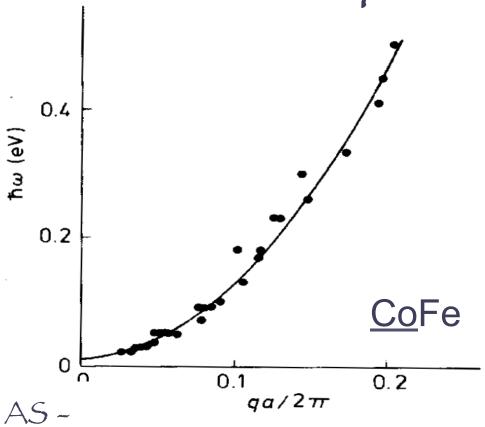
In half a century we have developed neutron scattering science enormously with an effective gain in source performance of only a factor of 4 !

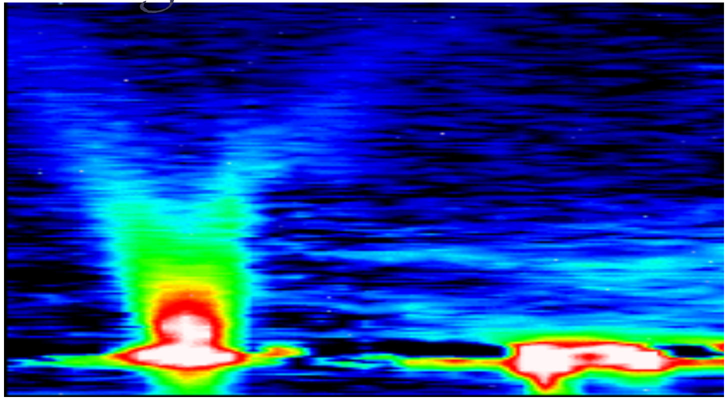
Cliff Shull – Neutron diffraction - showing where atoms are:





Bert Brockhouse – Spectroscopy - showing what atoms do:

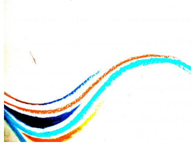




Using nowadays technique..

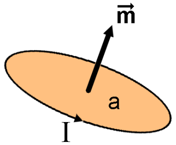
"Neutrons are beautiful !" By Sir Colin Windsor FRS

Wave



Particle

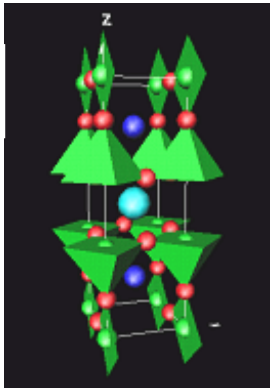
Magnetic moment



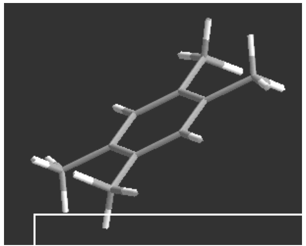
Neutral

Diffractometers - Measure structures

– Where atoms and molecules are 1 - 10 Ångström



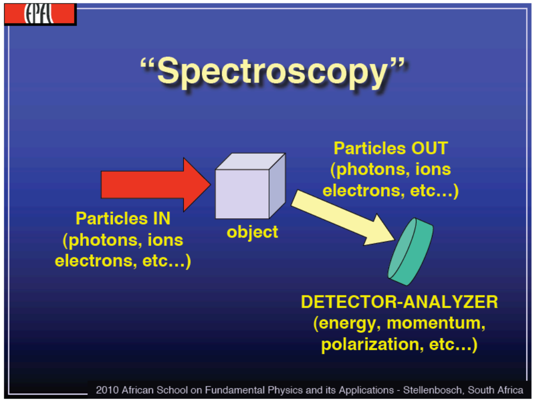
→ To analyze the structure of a material from the scattering pattern produced when a beam of radiation or particles (such as X-rays or neutrons) interacts with it



Spectrometers - Measure dynamics

– What atoms and molecules do 1 - 80 meV

→ To measure properties of light over a specific portion of the electromagnetic spectrum



"Spectroscopy"

Particles IN (photons, ions electrons, etc...)

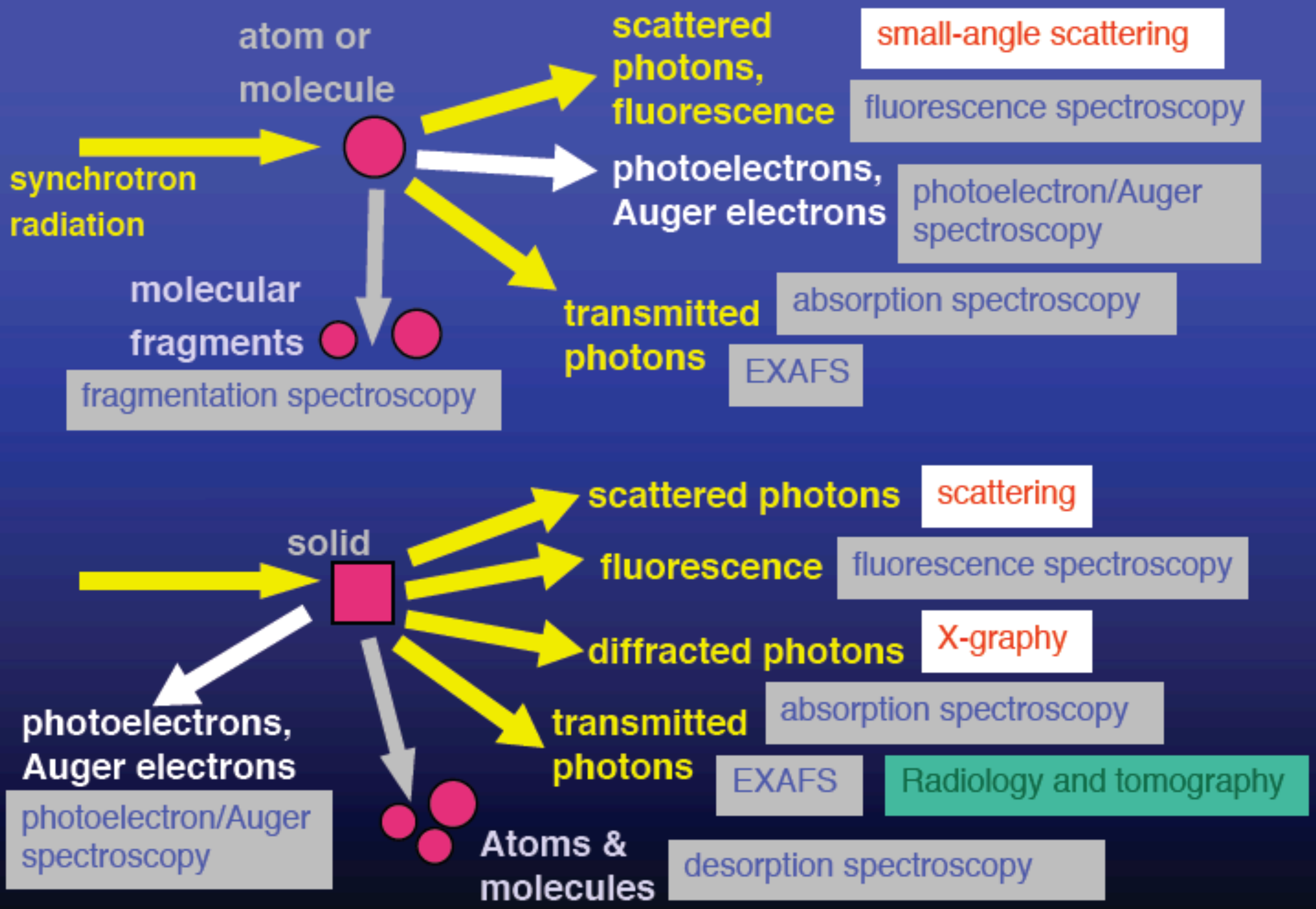
object

Particles OUT (photons, ions electrons, etc...)

DETECTOR-ANALYZER (energy, momentum, polarization, etc...)

2010 African School on Fundamental Physics and its Applications - Stellenbosch, South Africa

Three classes of experiments:



atom or molecule

synchrotron radiation

scattered photons, fluorescence

small-angle scattering

fluorescence spectroscopy

photoelectrons, Auger electrons

photoelectron/Auger spectroscopy

transmitted photons

absorption spectroscopy

EXAFS

molecular fragments

fragmentation spectroscopy

solid

scattered photons

scattering

fluorescence

fluorescence spectroscopy

diffracted photons

X-graphy

transmitted photons

absorption spectroscopy

EXAFS

Radiology and tomography

photoelectrons, Auger electrons

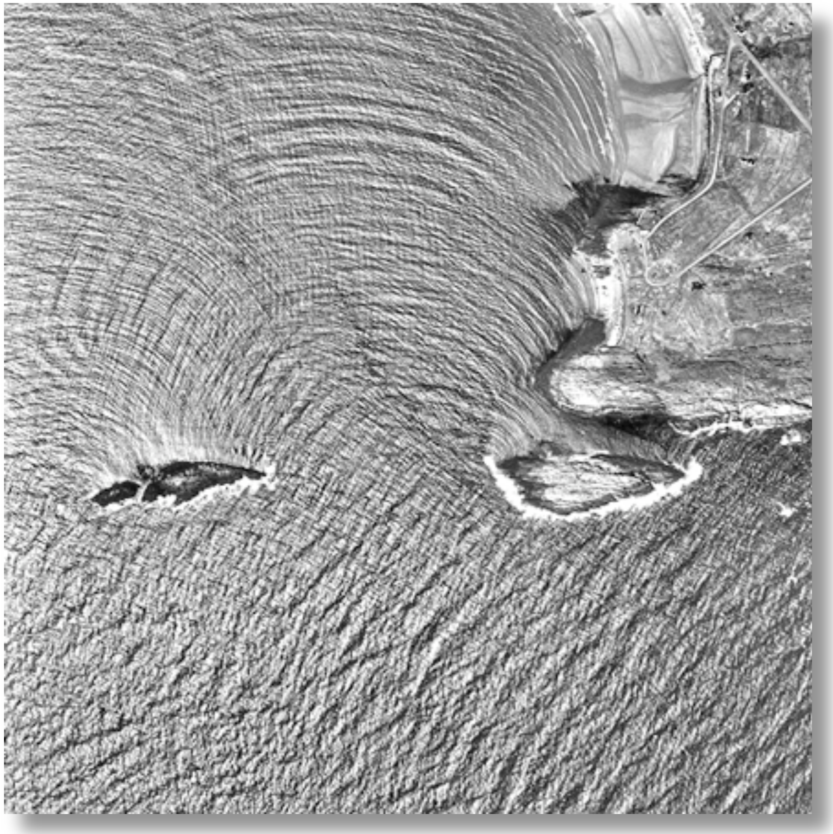
photoelectron/Auger spectroscopy

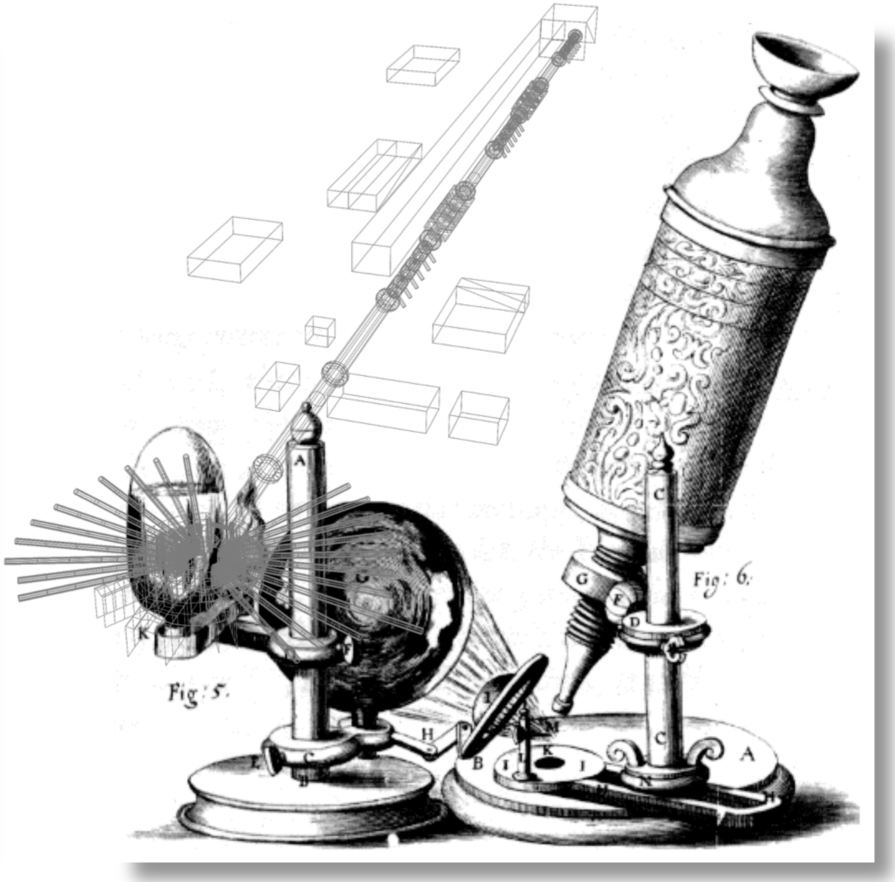
Atoms & molecules

desorption spectroscopy

X-Ray and Neutron beam

Complementarity between X-rays and Neutrons





Consider ESS/MaxIV equal in terms of functionality

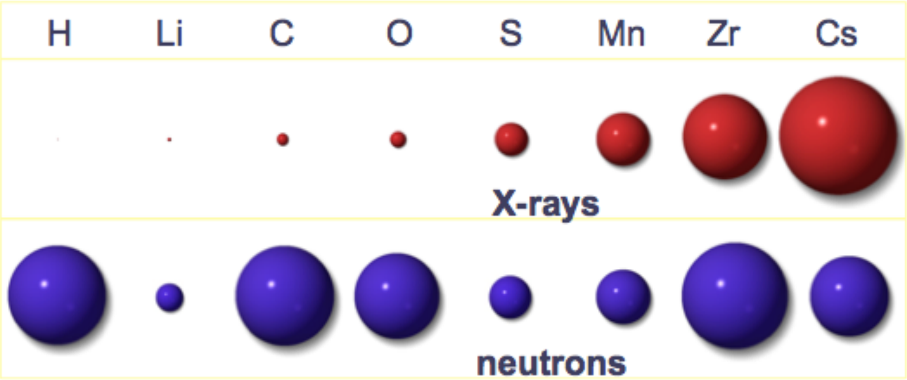
Complementarity between X-rays and Neutrons

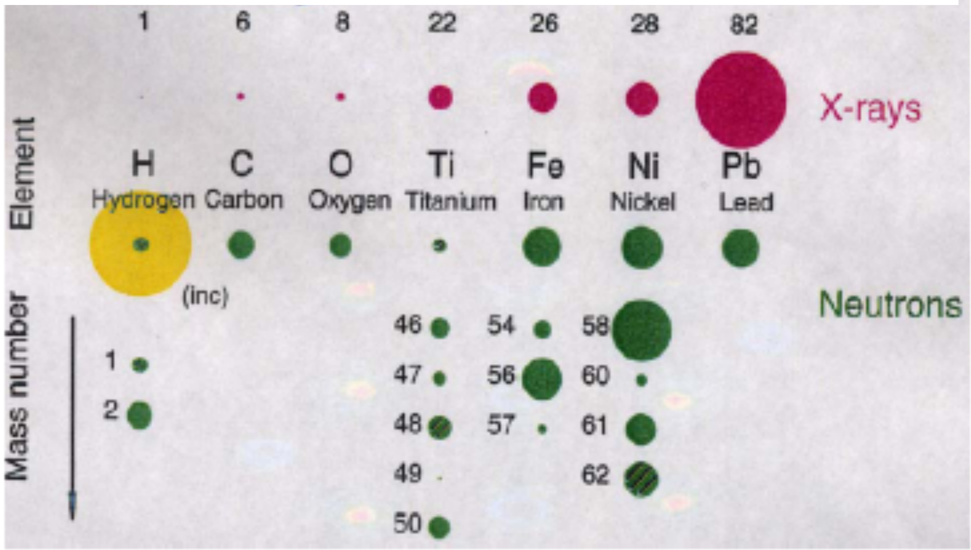
Neutrons	Synchrotron radiation
• Particle beam (neutral subatomic particle)	• Light beam (electromagnetic wave)
• Interactions with the nuclei and the magnetic moment of unpaired electrons (in the sample)	• Interactions with the electrons surrounding the nuclei (in the sample)
• Scattered by all elements, also the light ones like the hydrogen isotopes	• Mainly scattered by heavy elements
• Deep penetration depth (bulk studies of samples)	• Small penetration depth (surface studies of samples)
• Less intense beam measuring larger samples	• Very intense beam measuring small or ultra-dilute samples

Complementarity between X-rays and Neutrons

Neutrons Applications	SR Applications
Magnetic structures & excitations	Protein-crystal structures
Organic structures using the H-D isotope effect	Fast chemical reactions
Bulk studies (strains, excitations)	Surface studies (defects, corrosion)
Low-energy spectroscopy e.g. molecular vibrations	High-energy spectroscopy e.g. measurements of electron energy-levels

Complementarity between X-rays and Neutrons



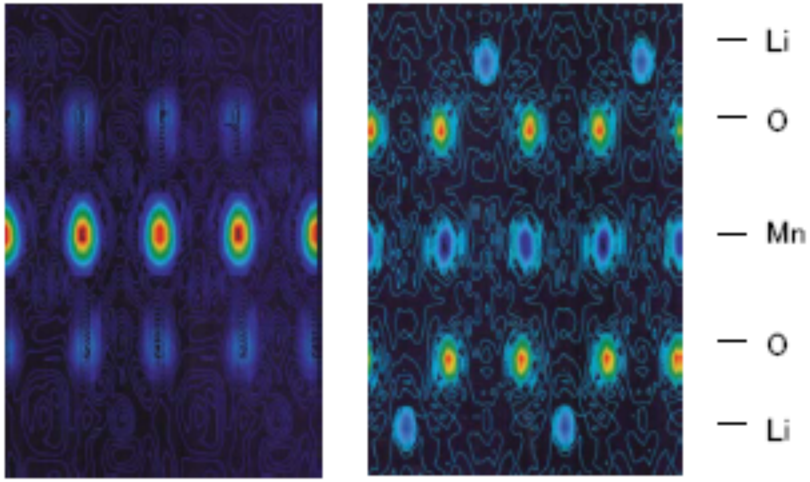


X-rays interact with electrons.

→ X-rays see high-Z atoms.

Neutrons interact with nuclei.

→ Neutrons see low-Z atoms.



Material for Li-battery seen by

X rays (left) and

Neutrons (right)

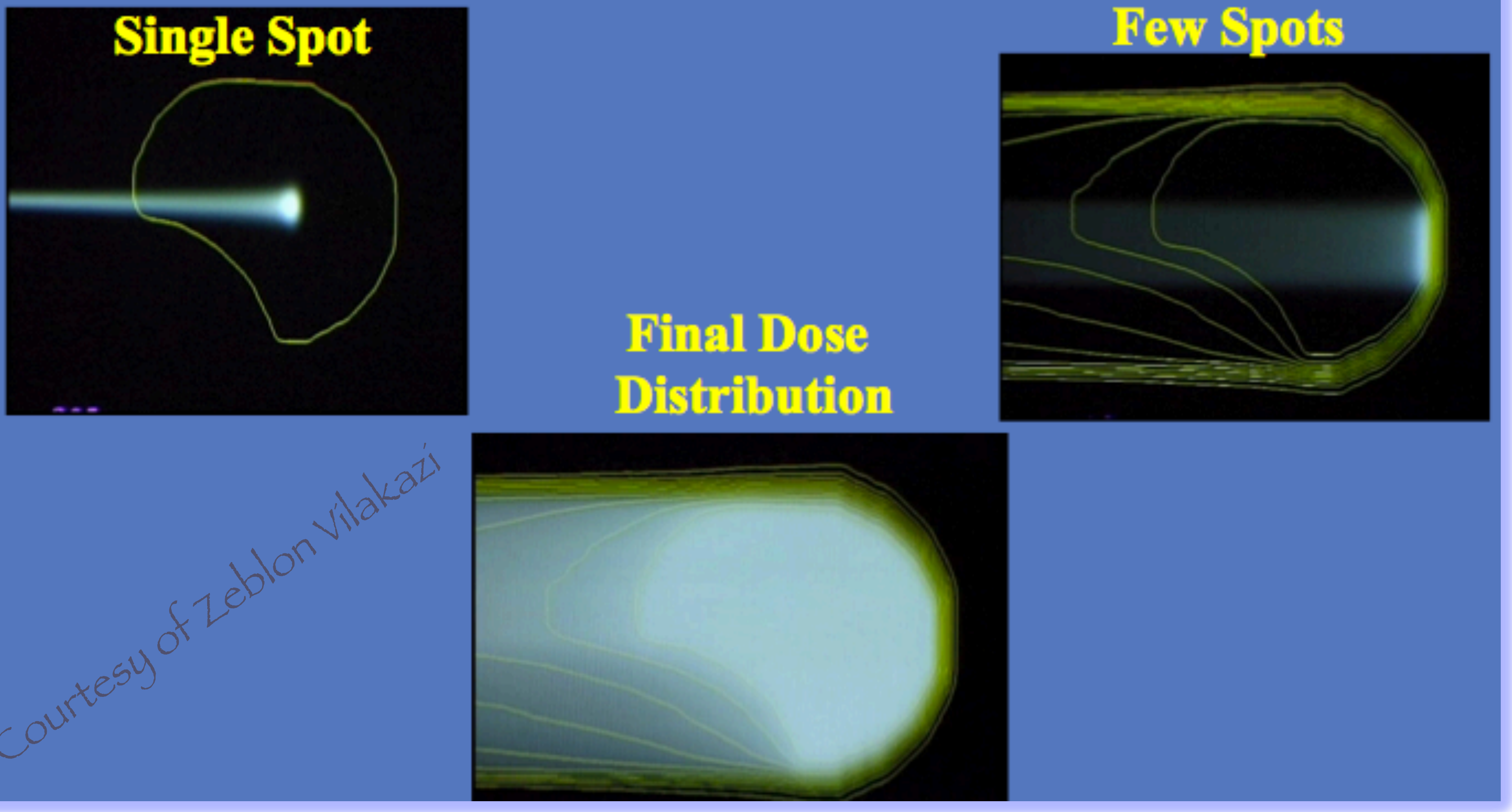
T. Kamiyama, et al.

iThemba Particle Therapy Centre [iTPTC]

NRF National Research Foundation

iThemba LABS Laboratory for Accelerator Based Sciences

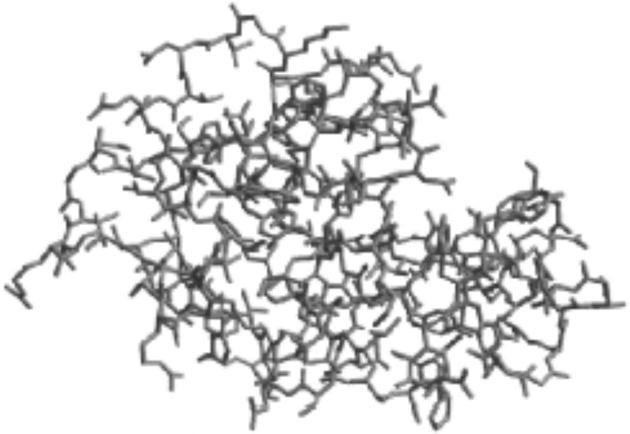
Spot Scanning Principle



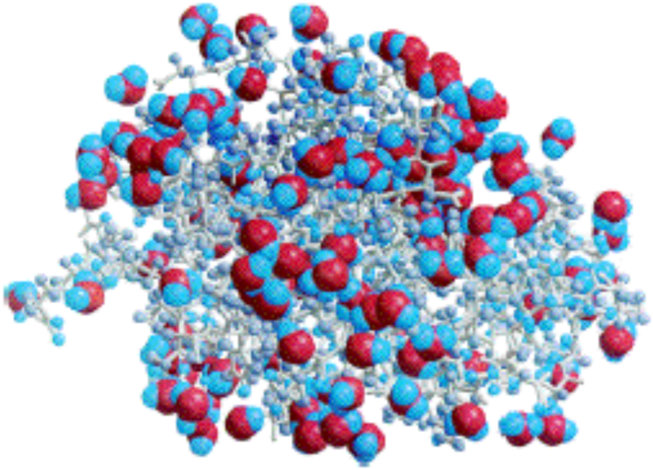
Courtesy of Zeblon Vilakazi

Complementarity between X-rays and Neutrons

Hen Egg-White Lysozyme



X-rays

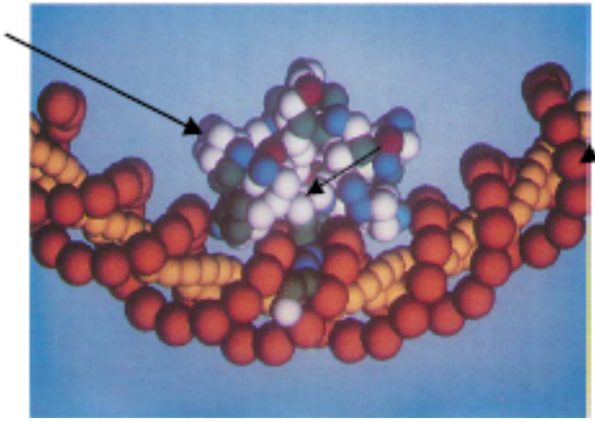


Neutrons

Water molecules Observed with neutrons

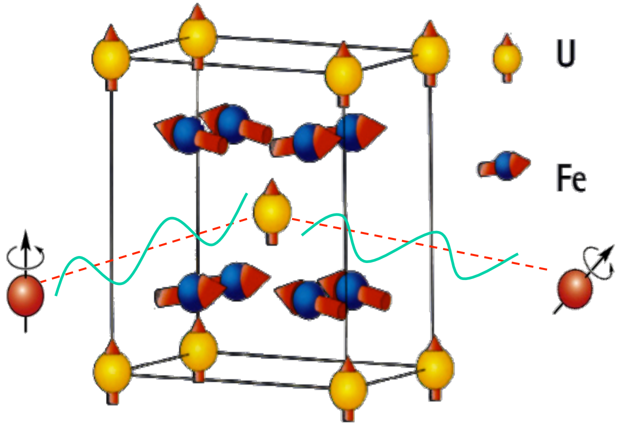
N. Niimura, et al.

From structure to function

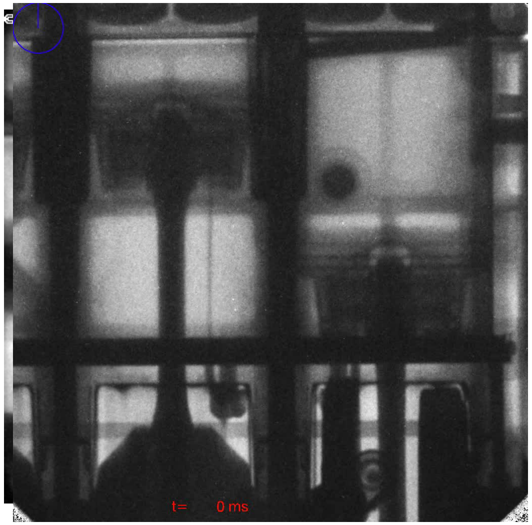


A proten molecule moving along theDNAchain

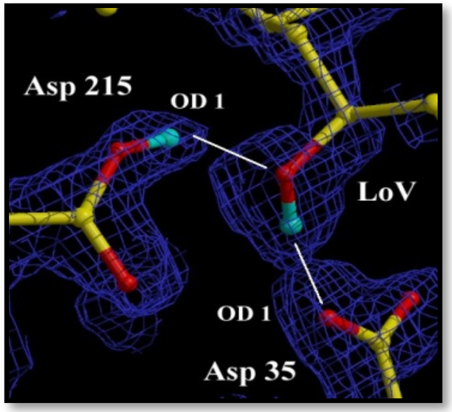
Neutrons and X-rays are complementary



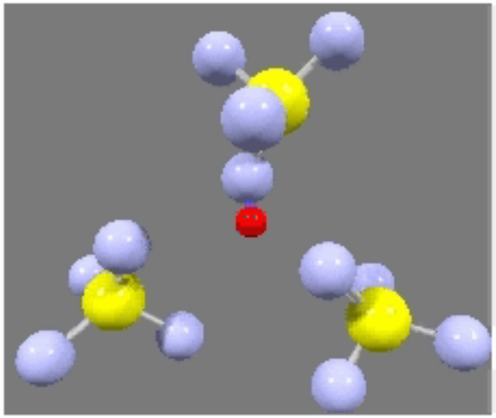
..see magnetic atoms



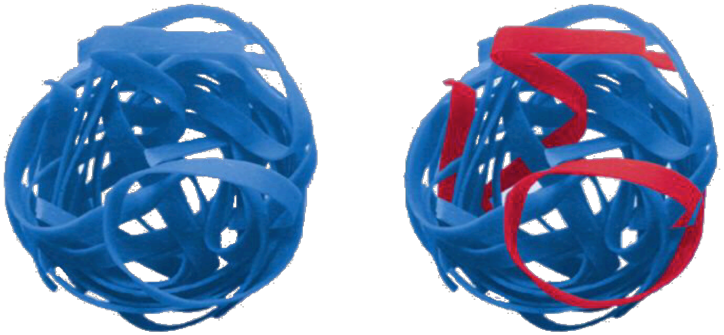
..see inside materials



..see light atoms



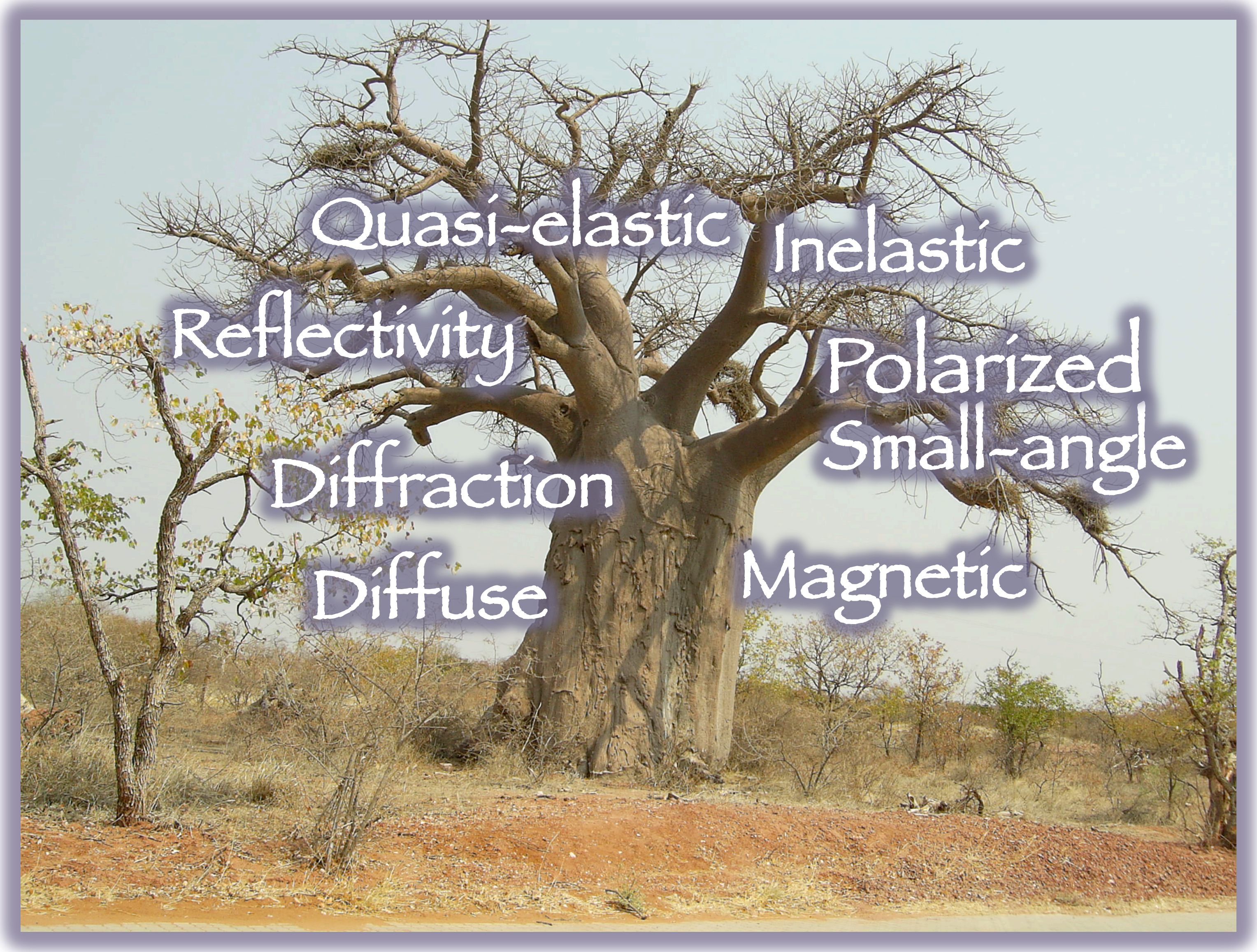
..see atoms move



..see isotopes

Scattering and Diffraction

Neutron Scattering Techniques



Isotope specific contrast

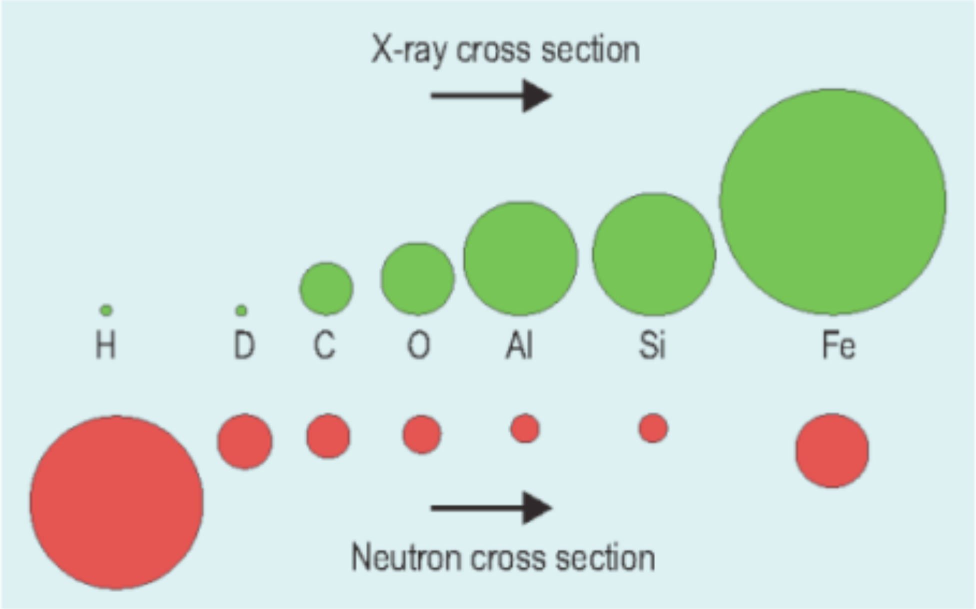
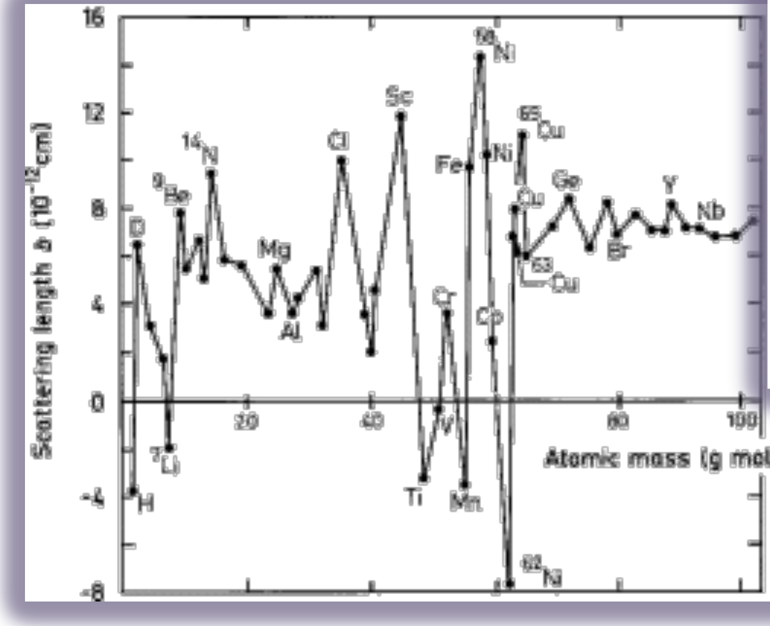


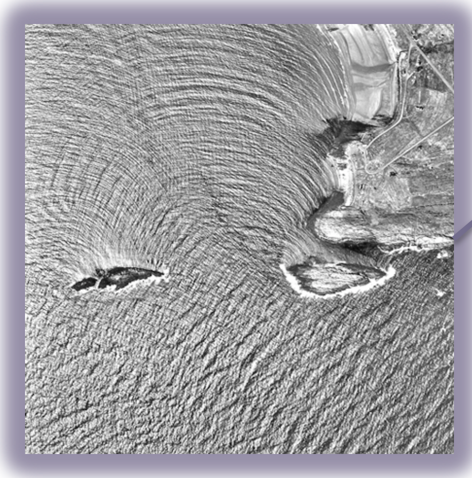
Fig. 2. Neutron and x-ray scattering cross-sections compared. Note that neutrons penetrate through Al much better than x rays do, yet are strongly scattered by hydrogen.

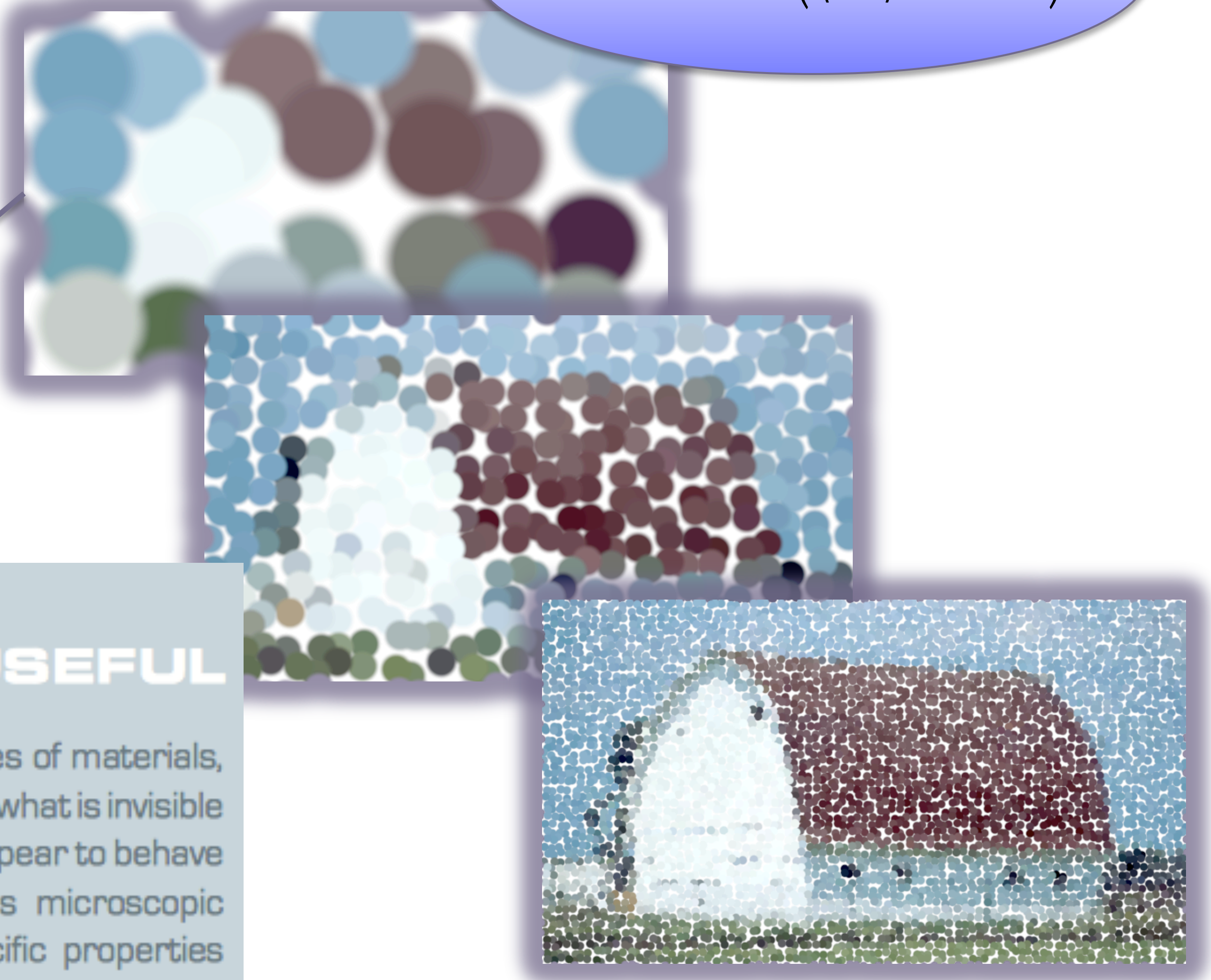


Scattering – coherence and incoherence

$$\sigma_{coh} = 4\pi\langle b\rangle^2$$

$$\sigma_{incoh} = 4\pi\left(\langle b^2\rangle - \langle b\rangle^2\right)$$





WHY NEUTRON SCATTERING IS USEFUL

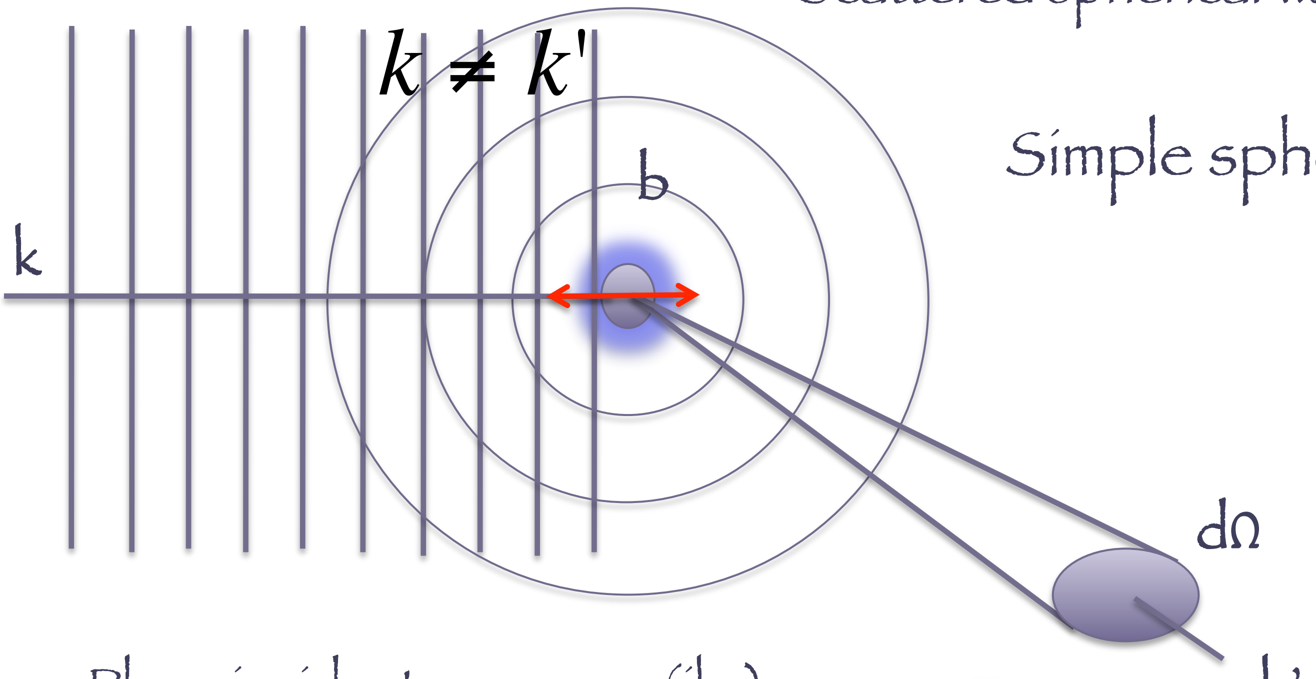
When used as a probe for small samples of materials, neutron beams have the power to reveal what is invisible using other radiations. Neutrons can appear to behave either as particles or as waves or as microscopic magnetic dipoles, and it is these specific properties which enable them to uncover information which is often impossible to access using other techniques.

Isotopes and spin?

Inelastic Scattering of plane wave

σ_{tot}=number of neutrons scattered in all directions per sec/incident flux

Scattered spherical wave: –b exp(ikr)/b



Simple spherical object!!

Plane incident wave: exp(ikr)

$$\left(\frac{d^2\sigma}{d\Omega\, dE}\right)$$

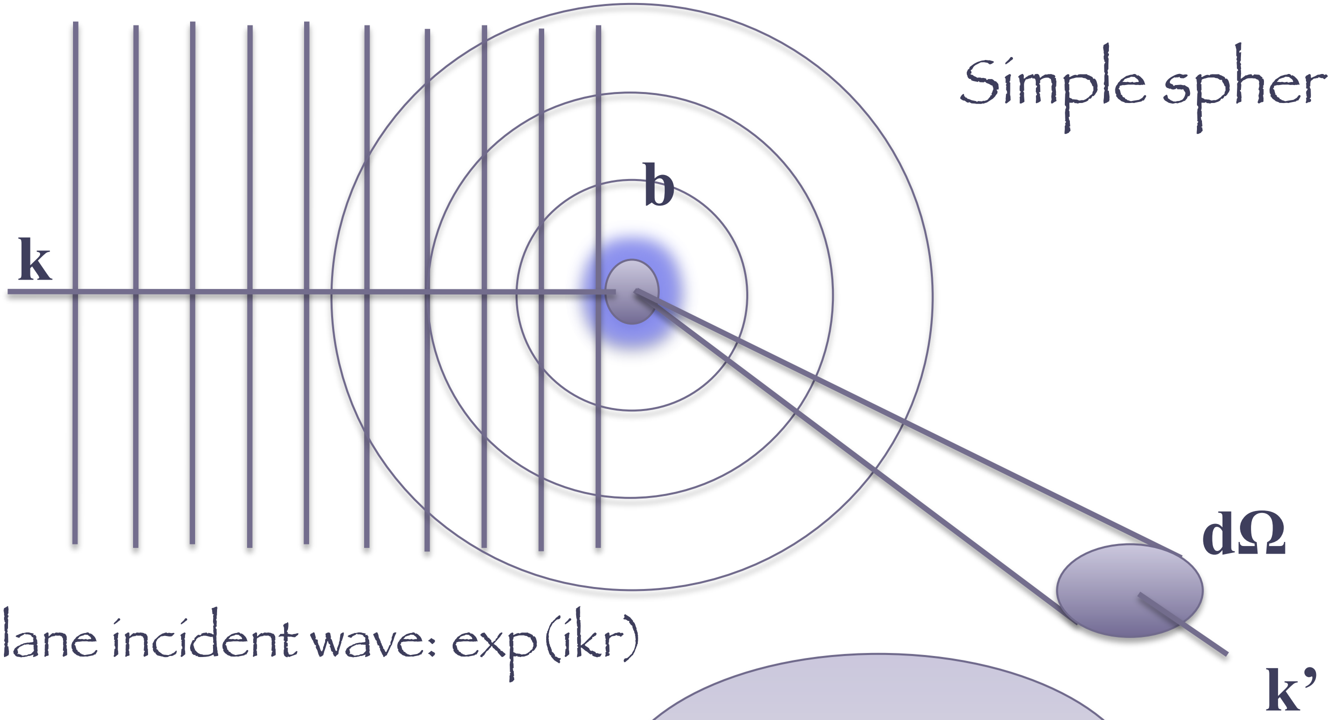
$$\sigma_{tot} = 4\pi b^2$$

Diffraction = Coherent Elastic Scattering of plane wave

σ_{tot}=number of neutrons scattered in all directions per sec/incident flux

Scattered spherical wave: –b exp(ikr)/b

Simple spherical object!!



Plane incident wave: exp(ikr)

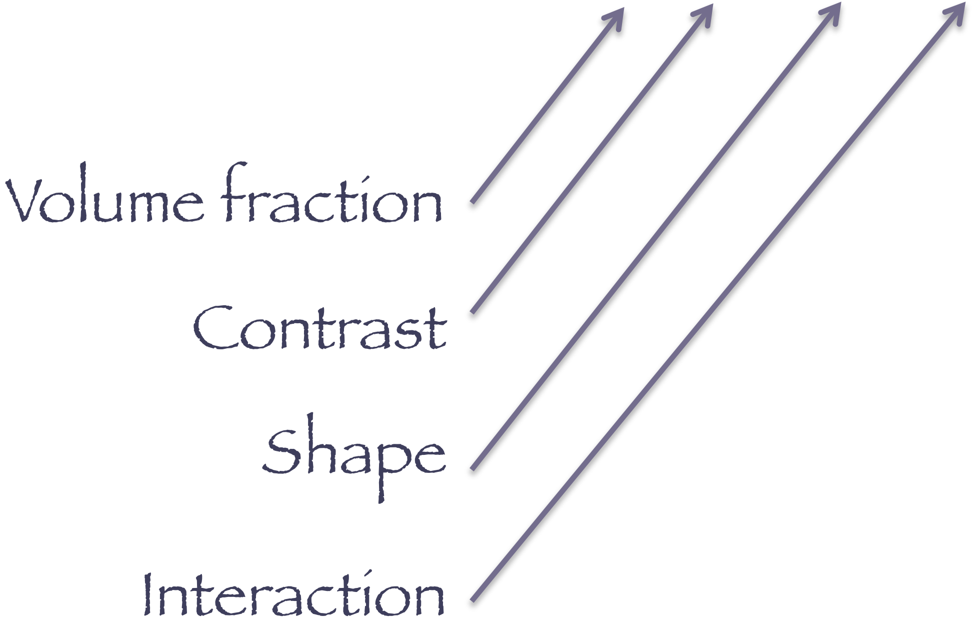
$$\sigma_{tot} = 4\pi b^2$$

$$\left(\frac{d\sigma}{d\Omega}\right), \left(\frac{d^2\sigma}{d\Omega\, dE}\right)$$

Scattering

- **Cross section:** $d\sigma = \dfrac{(\#\ \text{particles scattered into solid angle } \Delta\Omega/\text{s})}{(\#\ \text{particles incident/sec})(\#\ \text{scattering centers/area})}$

$$\frac{d\sigma(Q)}{d\Omega} = N_p V_p \overline{\rho} P(Q) S(Q)$$



Volume fraction

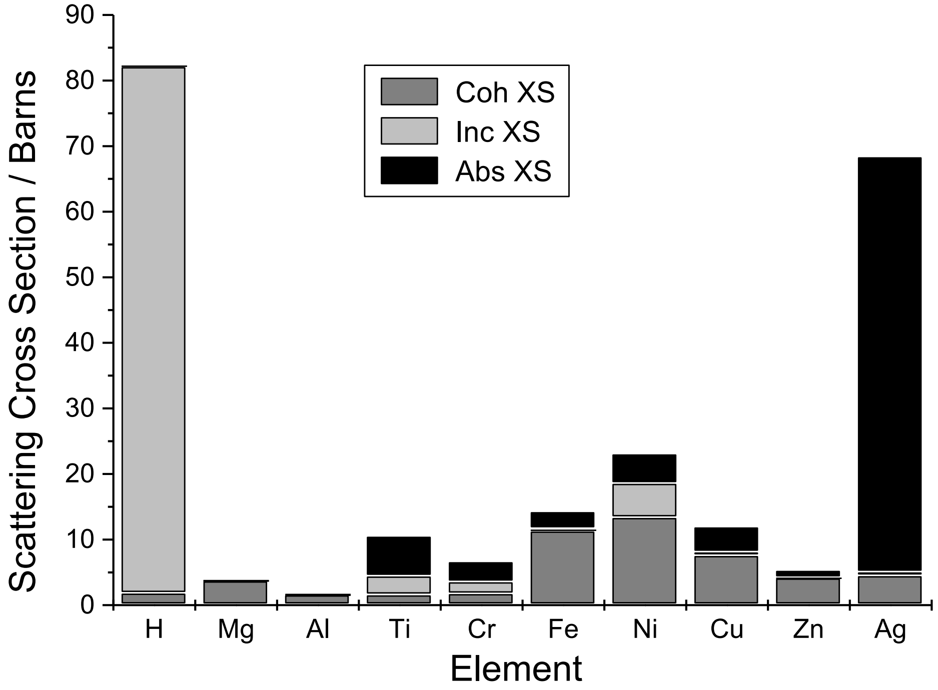
Contrast

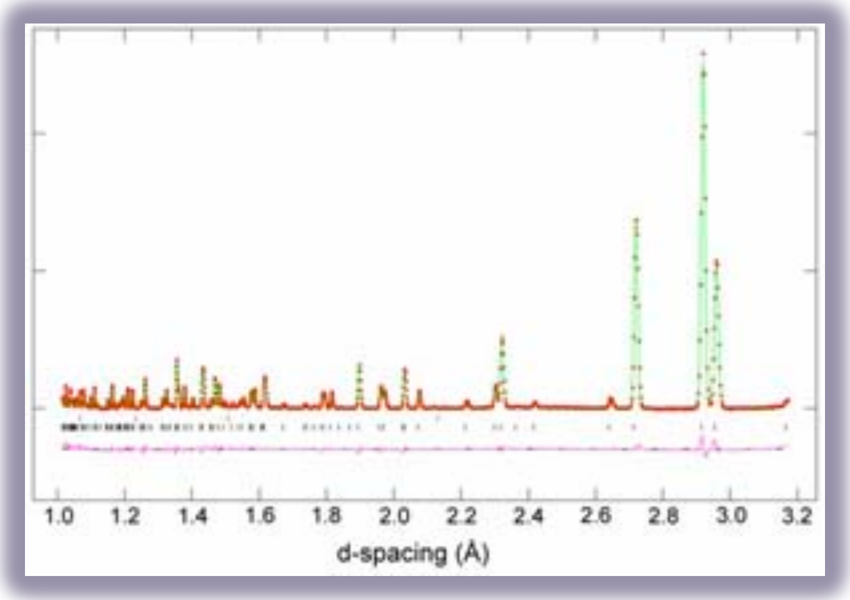
Shape

Interaction

Neutron Scattering XS

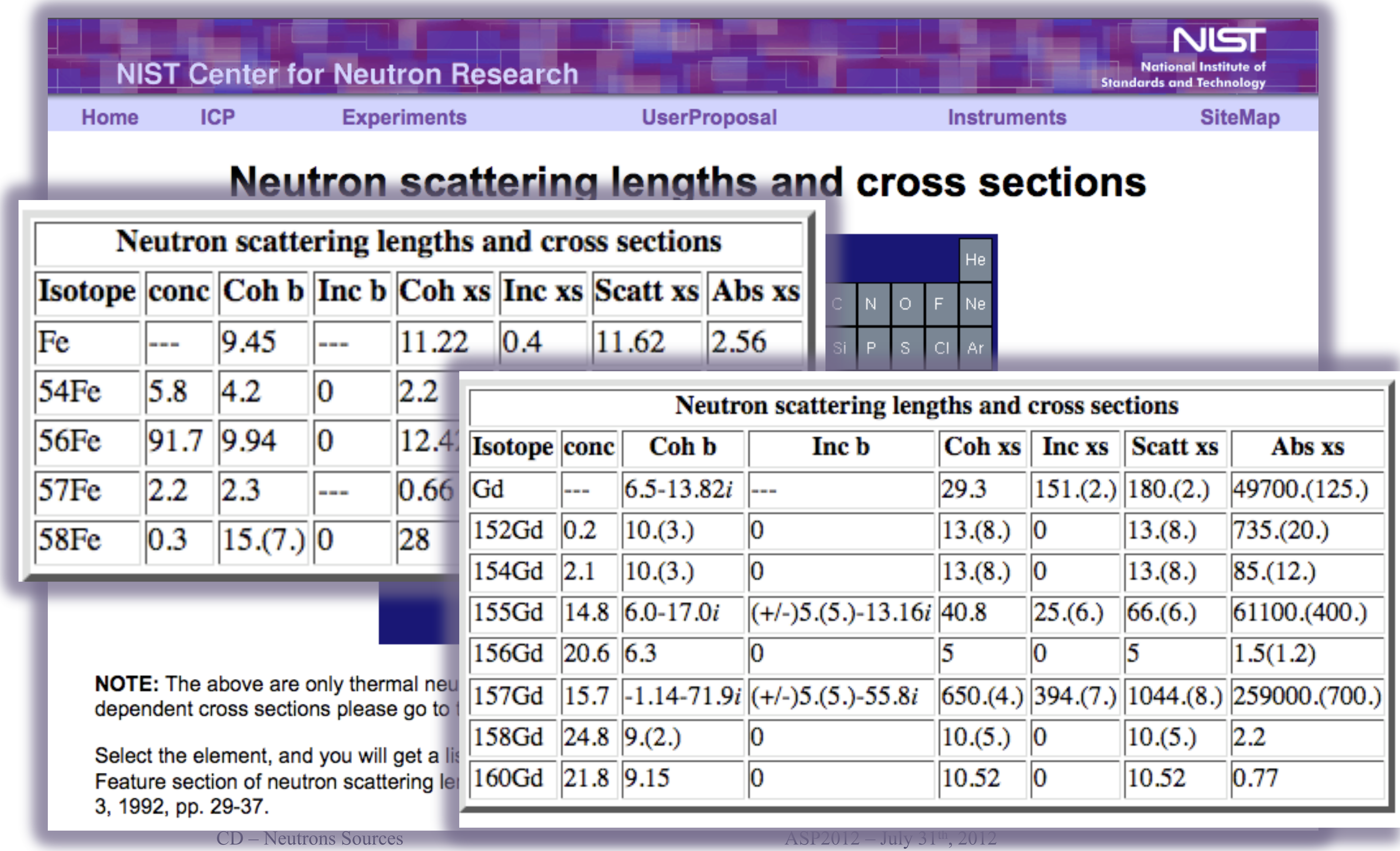
Coherent XS~ Signal
Incoherent XS~ Background
Absorption XS~1/Intensity





The neutron diffraction pattern of sulfuric acid tetrahydrate at 4.2 K as seen by the 90 degree detectors on HRPD, and fitted with the existing X-ray derived structural model for the deuterated species.

Neutron cross sections



NIST Center for Neutron Research

Neutron scattering lengths and cross sections

Neutron scattering lengths and cross sections

Isotope	conc	Coh b	Inc b	Coh xs	Inc xs	Scatt xs	Abs xs
Fe	---	9.45	---	11.22	0.4	11.62	2.56
54Fe	5.8	4.2	0	2.2			
56Fe	91.7	9.94	0	12.4			
57Fe	2.2	2.3	---	0.66			
58Fe	0.3	15.(7.)	0	28			

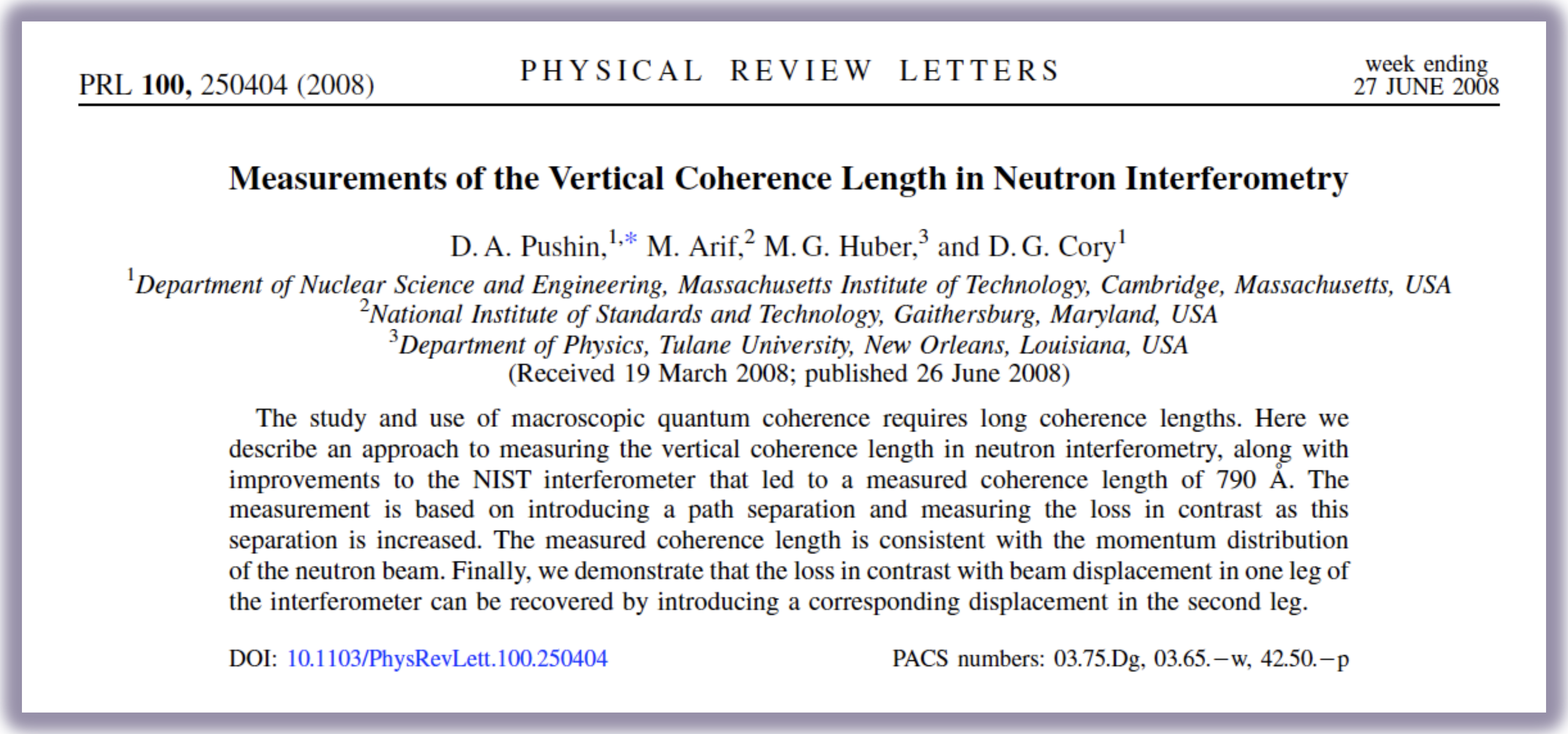
Neutron scattering lengths and cross sections

Isotope	conc	Coh b	Inc b	Coh xs	Inc xs	Scatt xs	Abs xs
Gd	---	6.5-13.82*i*	---	29.3	151.(2.)	180.(2.)	49700.(125.)
152Gd	0.2	10.(3.)	0	13.(8.)	0	13.(8.)	735.(20.)
154Gd	2.1	10.(3.)	0	13.(8.)	0	13.(8.)	85.(12.)
155Gd	14.8	6.0-17.0*i*	(+/-)5.(5.)-13.16*i*	40.8	25.(6.)	66.(6.)	61100.(400.)
156Gd	20.6	6.3	0	5	0	5	1.5(1.2)
157Gd	15.7	-1.14-71.9*i*	(+/-)5.(5.)-55.8*i*	650.(4.)	394.(7.)	1044.(8.)	259000.(700.)
158Gd	24.8	9.(2.)	0	10.(5.)	0	10.(5.)	2.2
160Gd	21.8	9.15	0	10.52	0	10.52	0.77

NOTE: The above are only thermal neu
dependent cross sections please go to t

Select the element, and you will get a lis
Feature section of neutron scattering le
3, 1992, pp. 29-37.

Neutron Coherency Length



PRL **100,** 250404 (2008) PHYSICAL REVIEW LETTERS week ending
27 JUNE 2008

Measurements of the Vertical Coherence Length in Neutron Interferometry

D. A. Pushin,[1,*] M. Arif,[2] M. G. Huber,[3] and D. G. Cory[1]
[1]*Department of Nuclear Science and Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts, USA*
[2]*National Institute of Standards and Technology, Gaithersburg, Maryland, USA*
[3]*Department of Physics, Tulane University, New Orleans, Louisiana, USA*

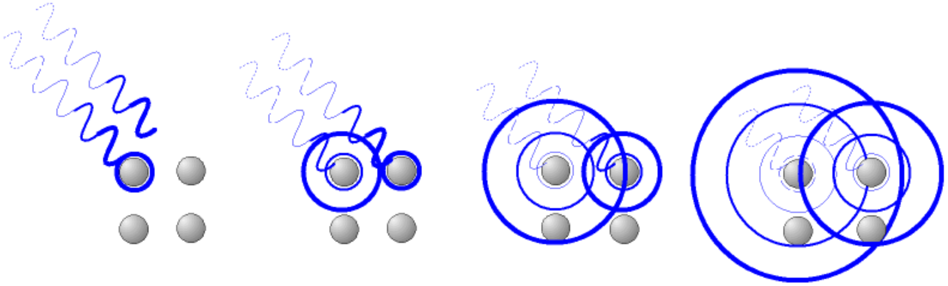
(Received 19 March 2008; published 26 June 2008)

The study and use of macroscopic quantum coherence requires long coherence lengths. Here we describe an approach to measuring the vertical coherence length in neutron interferometry, along with improvements to the NIST interferometer that led to a measured coherence length of 790 Å. The measurement is based on introducing a path separation and measuring the loss in contrast as this separation is increased. The measured coherence length is consistent with the momentum distribution of the neutron beam. Finally, we demonstrate that the loss in contrast with beam displacement in one leg of the interferometer can be recovered by introducing a corresponding displacement in the second leg.

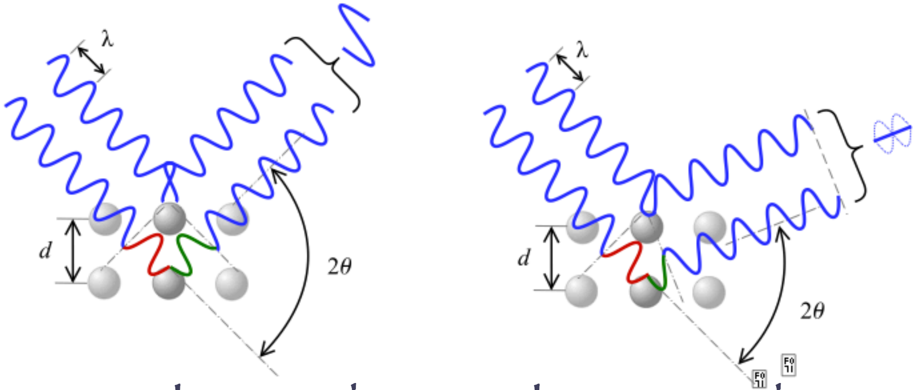
DOI: 10.1103/PhysRevLett.100.250404 PACS numbers: 03.75.Dg, 03.65.−w, 42.50.−p

Diffraction - Bragg

Diffraction of X-rays or neutrons by polycrystalline samples is one of the most important, powerful and widely used analytical techniques available to materials scientists. For most crystalline substances of technological importance, the bulk properties of a powder or a polycrystalline solid, averaged throughout the sample, are required; in general a single-crystal data, even if they can be obtained, are usually of little interest except for determination of the crystal structure or for studying some other fundamental physical property. By *J Ian Langford and Daniel Louer*



X-rays interact with the atoms in a crystal.

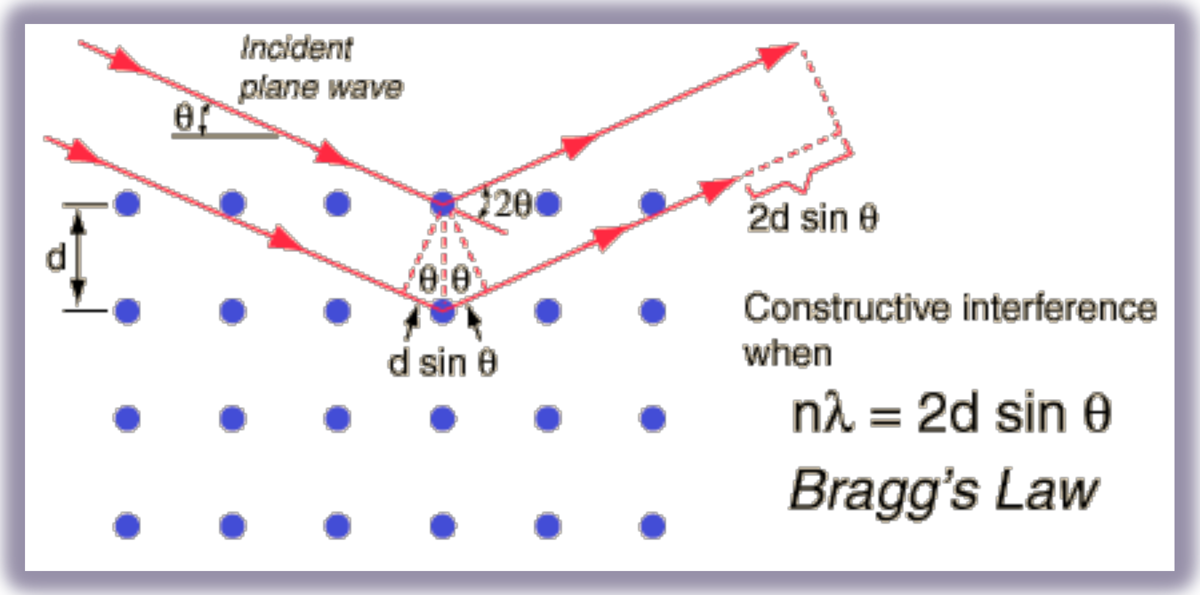


According to the 2θ deviation, the phase shift causes constructive (left figure) or destructive (right figure) interferences.

Diffraction - Bragg

- Bragg / Laue scattering
- Coherent elastic scattering

Two beams with identical wavelength and phase approach a crystalline solid and are scattered off two different atoms within it. The lower beam traverses an extra length of 2dsin θ . Constructive interference occurs when this length is equal to an integer multiple of the wavelength of the radiation.



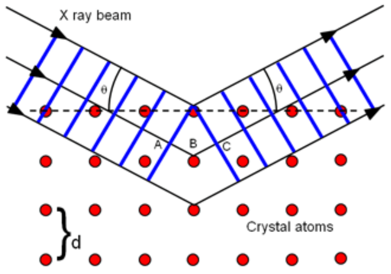
Constructive interference when

$$n\lambda = 2d \sin \theta$$

Bragg's Law

Diffraction - Bragg

Using the grains as internal strain gauges



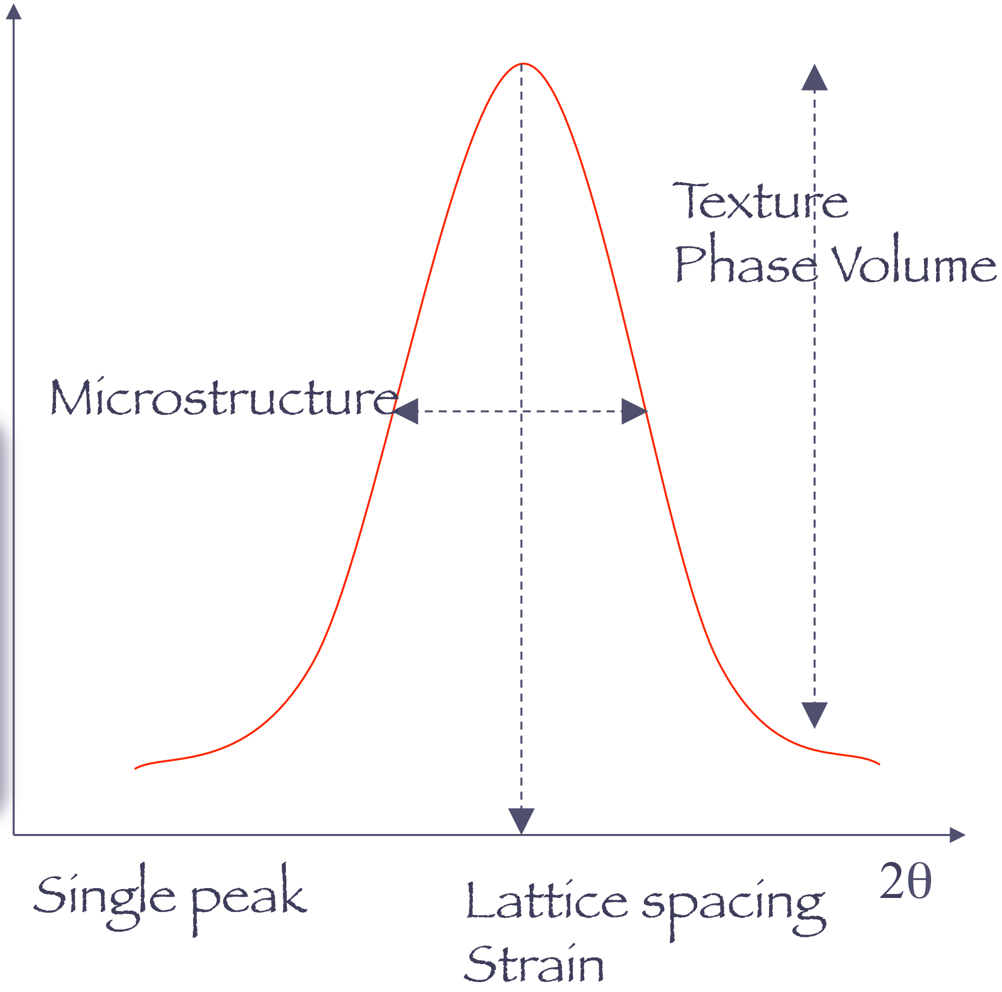
$$\lambda = 2d\sin\theta$$

$$\varepsilon = -\cot(\theta)\,(\theta - \theta_0)$$

Two ways to measure d:

-keep λ fixed and measure θ
constant wavelength

-keep θ fixed and measure λ
time-of-flight

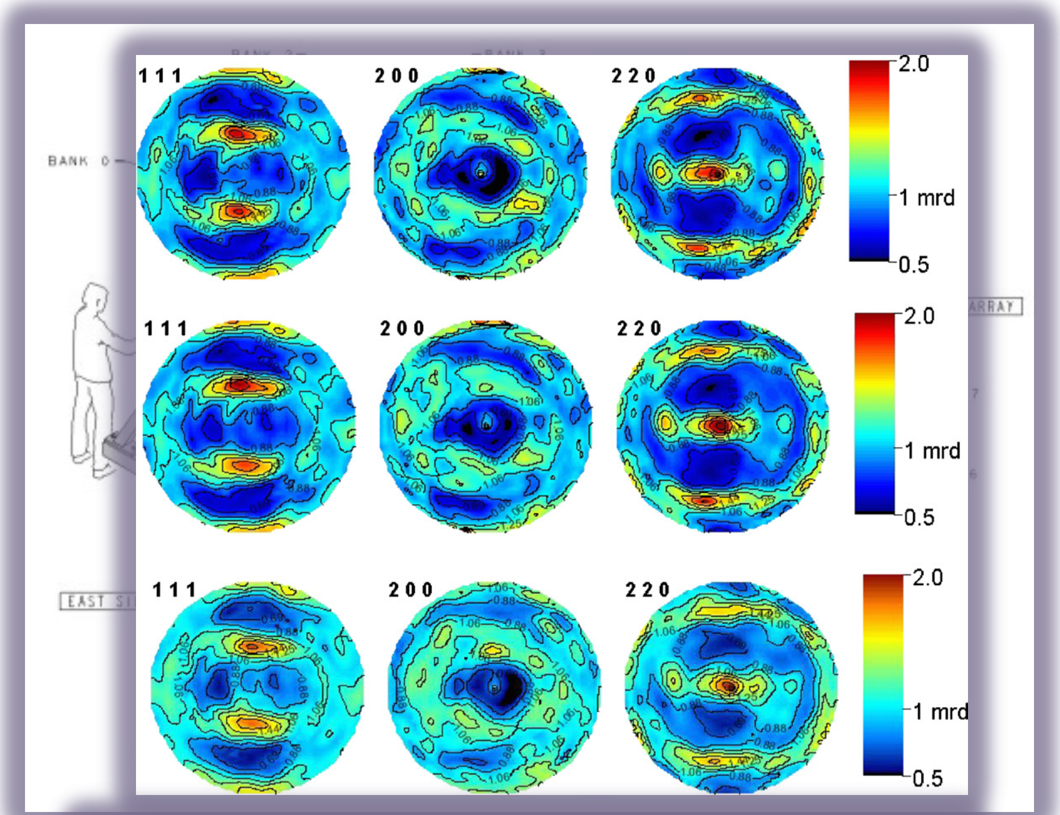


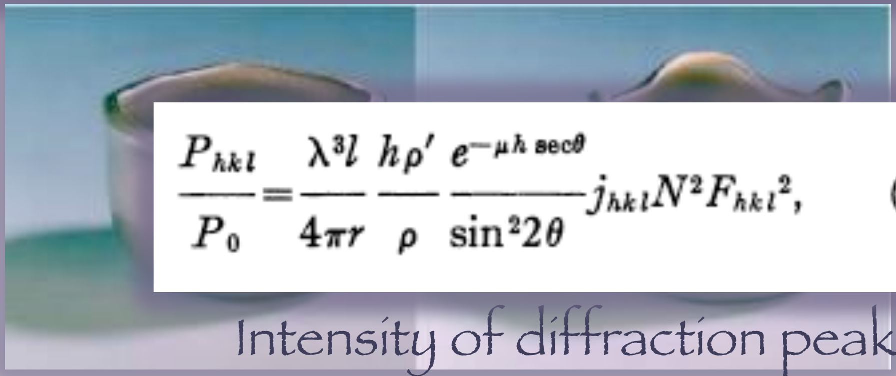
Diffraction: Texture

- ISIS: GEM instrument
- Near 4π coverage

Example:

- Cold rolled copper, simulating manufacturing process for archeometry
- 2mm thick disks
- 20x20mm^2 beam
- 2 min counting times



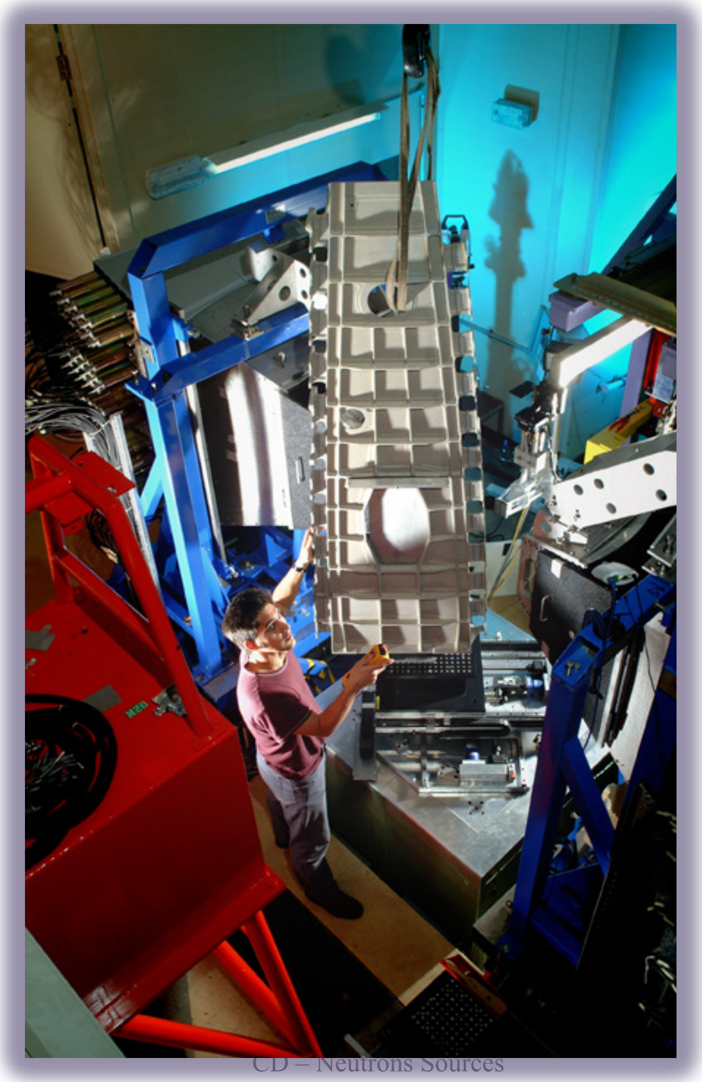


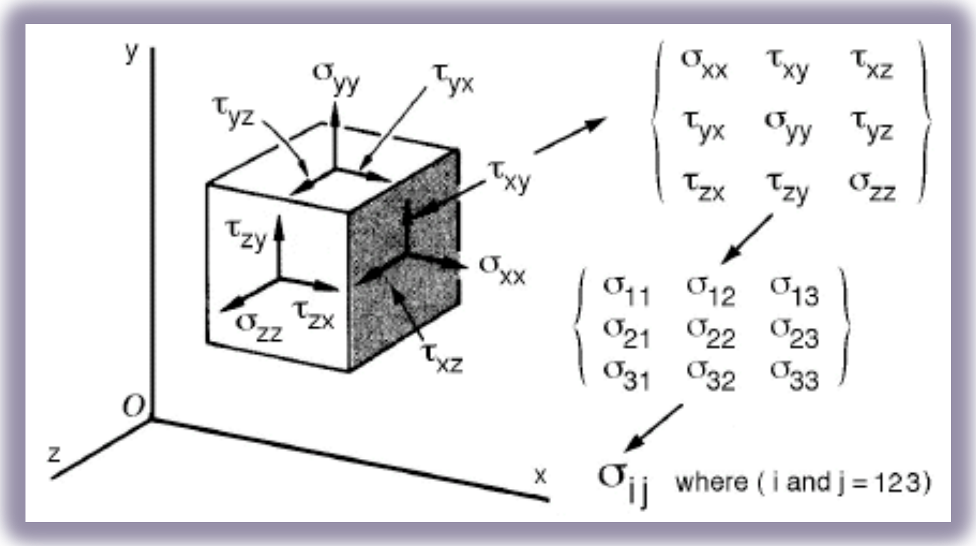
$$\frac{P_{hkl}}{P_0}=\frac{\lambda^3 l}{4\pi r}\,\frac{h\rho'}{\rho}\,\frac{e^{-\mu h\sec\theta}}{\sin^2 2\theta}\,j_{hkl}N^2F_{hkl}^2, \qquad (15)$$

Intensity of diffraction peak

Neutron texture analysis on GEM at ISIS
W. Kockelmann, L.C. Chapon and P.G. Radaelli
Physica B, Vol. 385-386 (1), pp639-643 (2006)

Diffraction: Stress and Strain

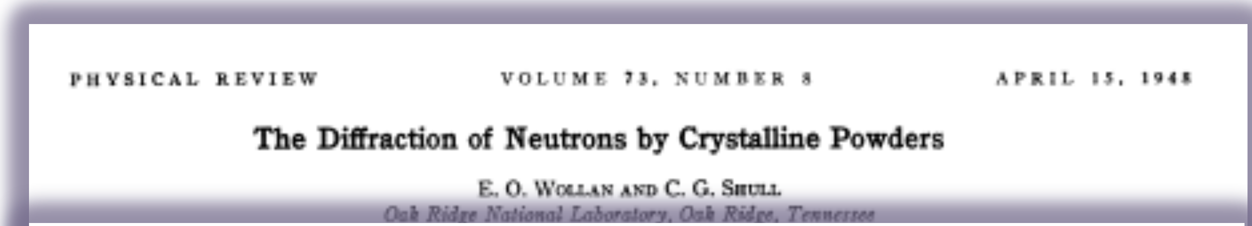




Applications:

Residual stresses
Fatigue/Structural
Integrity
Welds
Alloy development
Microstructure/Texture
Phase transformation
In-situ experiments

Example - Diffraction

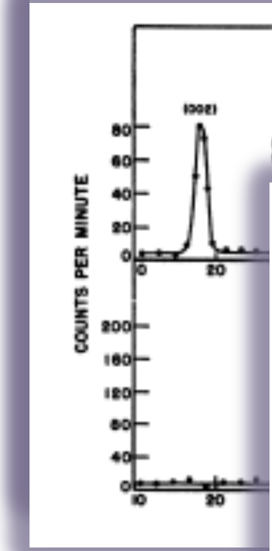


PHYSICAL REVIEW VOLUME 73, NUMBER 8 APRIL 15, 1948

The Diffraction of Neutrons by Crystalline Powders

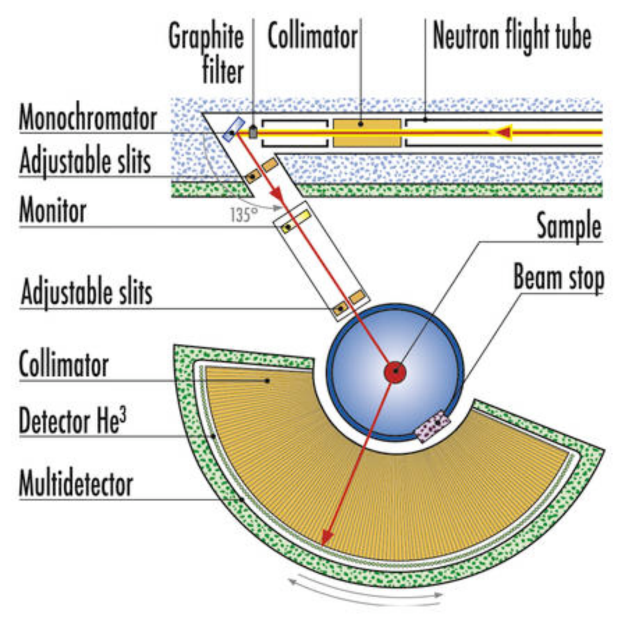
E. O. Wollan and C. G. Shull

Oak Ridge National Laboratory, Oak Ridge, Tennessee

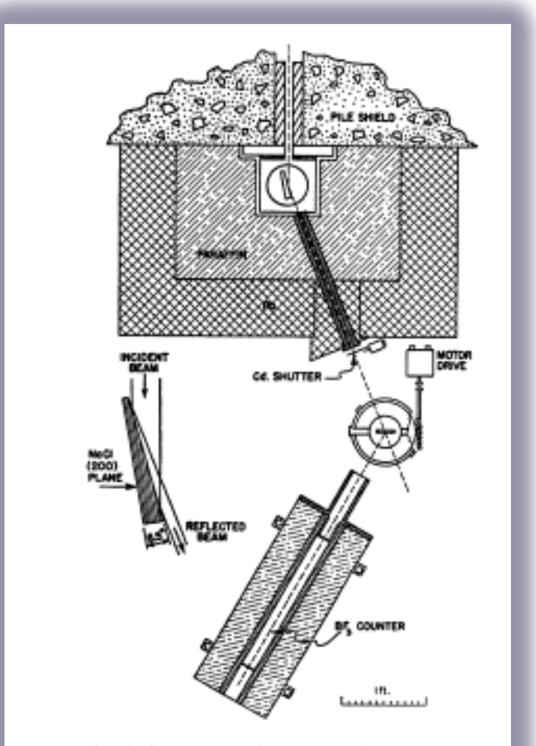


P

Fɪɢ. 3. Powder diffraction pat-
erns for diamond and graphite.
he major part of the diffuse
cattering in these patterns
rises from multiple scattering
the samples.



D2B at the ILL, Grenoble, 50 years later

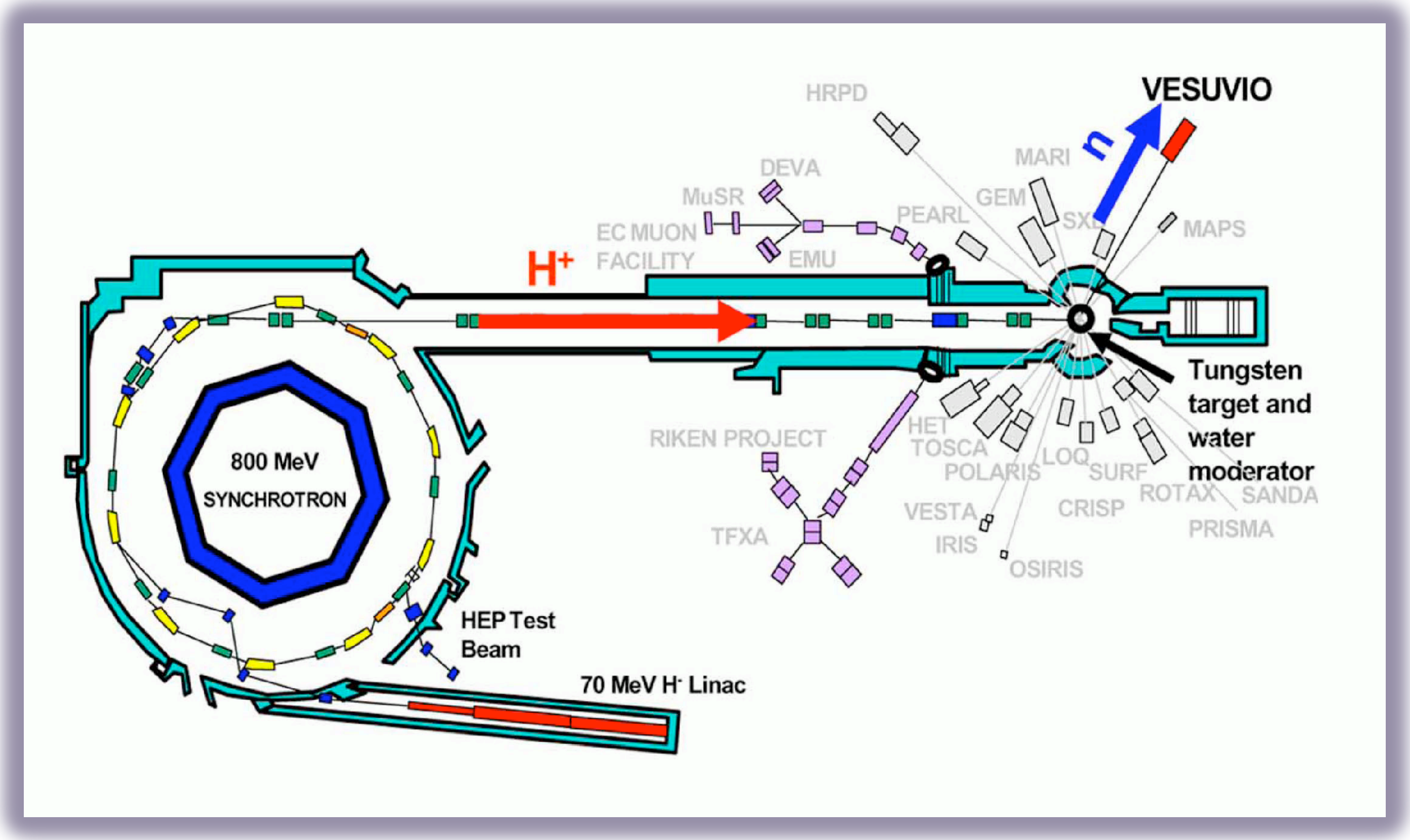


Fɪɢ. 1. Arrangement of apparatus, showing the mono-chromating crystal (detailed in left center) collimating slits, shielding, second spectrometer with location of powder specimen and counter.

$$\frac{P_{hkl}}{P_0}=\frac{\lambda^3 l}{4\pi r}\,\frac{h\rho'}{\rho}\,\frac{e^{-\mu h\sec\theta}}{\sin^2 2\theta}\,j_{hkl}N^2F_{hkl}^2, \qquad (15)$$

Intensity of diffraction peak

Spallation Sources: Time of Flight



Fast, short-wavelength neutrons arrive earlier at detector!

$$\lambda = \frac{h}{p} = \frac{h}{mv} = \frac{ht}{mL}$$

De Broglie

+

$$\lambda = 2d\sin\theta$$

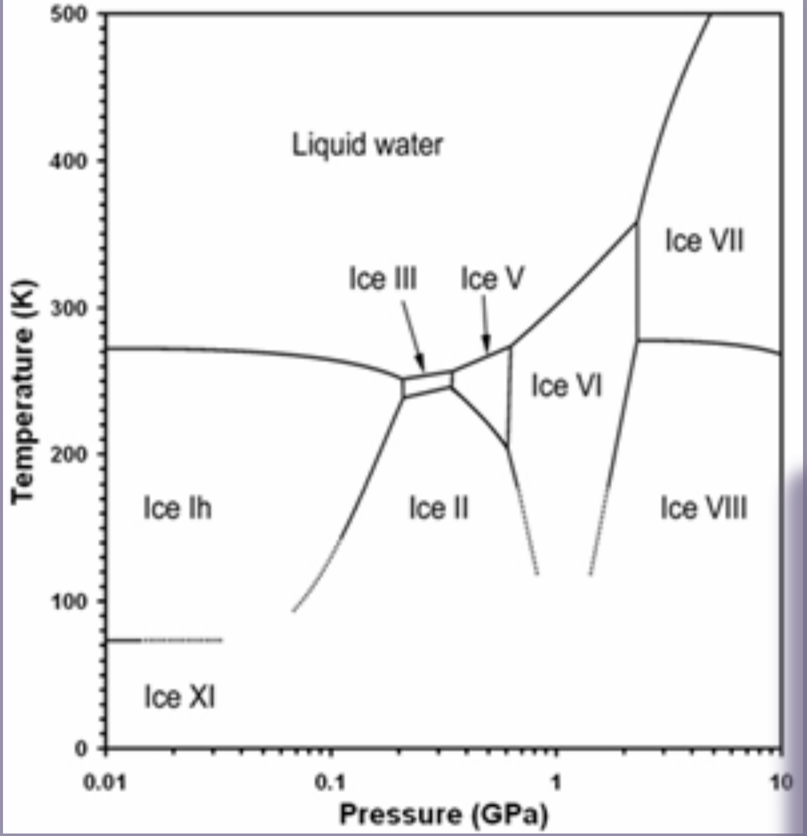
Bragg

=

Time-of-Flight:

$$d = \frac{h}{2mL\sin\theta}t$$

Ice!!



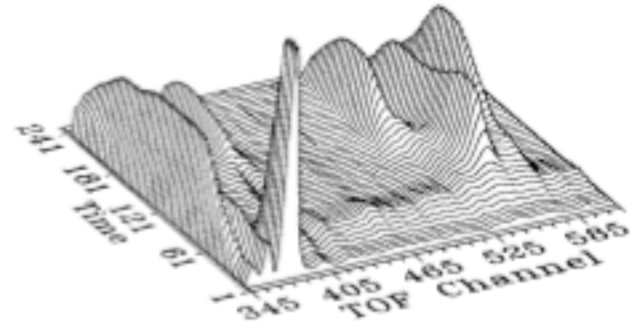


Figure 1. Neutron diffraction patterns measured in the course of heating of the recovered D_2O high-pressure phase ice VIII from 94 to 273 K.

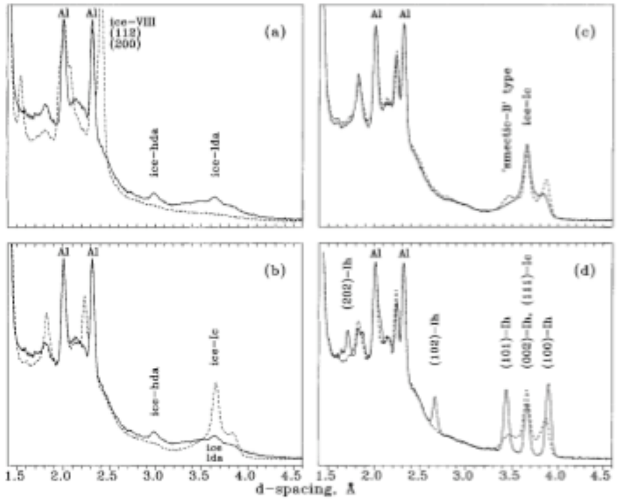


Figure 2. Neutron diffraction patterns of D_2O ices before and after phase transitions: (a) from ice VIII (dashed line) to a mixture of hda + lda ices (solid line) at 125 K; (b) from the mixture of hda + lda ices (solid line) to ice Ic (dashed line) at 160 K; (c) from ice Ic (solid line) to the hexagonal phase, "smectic B" type structure (dashed line), at 190 K; (d) from "smectic B" type ice (dashed line) to ice Ih (solid line) at 230 K. The diffraction patterns also contain peaks from the aluminum sample can and cryostat.

Batteries

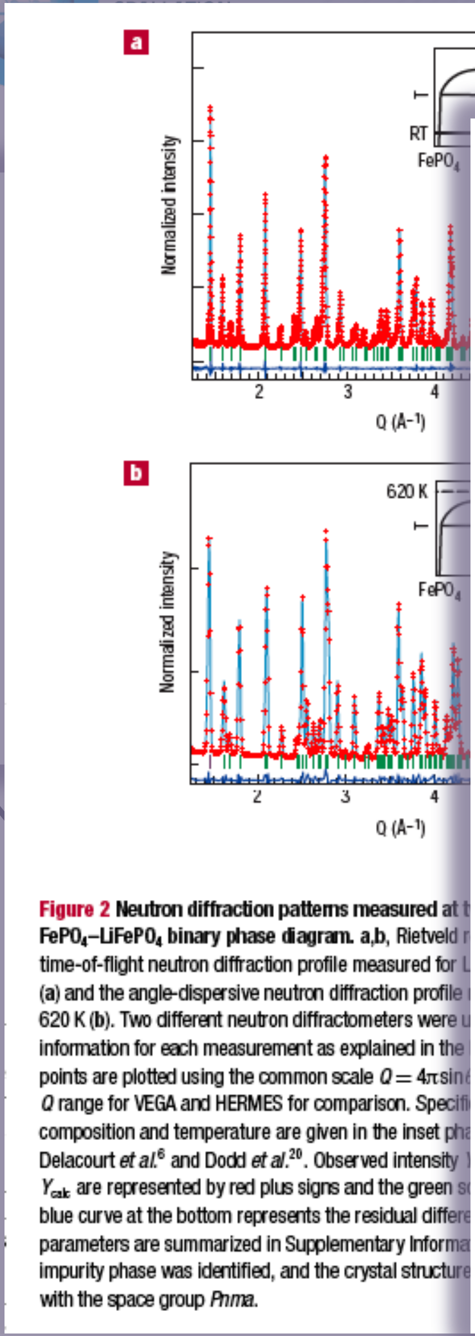


Figure 2 **Neutron diffraction patterns measured at t**
FePO$_4$–LiFePO$_4$ binary phase diagram. a,b, Rietveld r
time-of-flight neutron diffraction profile measured for L
(a) and the angle-dispersive neutron diffraction profile
620 K (b). Two different neutron diffractometers were u
information for each measurement as explained in the
points are plotted using the common scale $Q = 4\pi\sin$
Q range for VEGA and HERMES for comparison. Specifi
composition and temperature are given in the inset pha
Delacourt *et al.*[6] and Dodd *et al.*[20]. Observed intensity
Y_{calc} are represented by red plus signs and the green s
blue curve at the bottom represents the residual differe
parameters are summarized in Supplementary Informa
impurity phase was identified, and the crystal structure
with the space group *Pnma*.

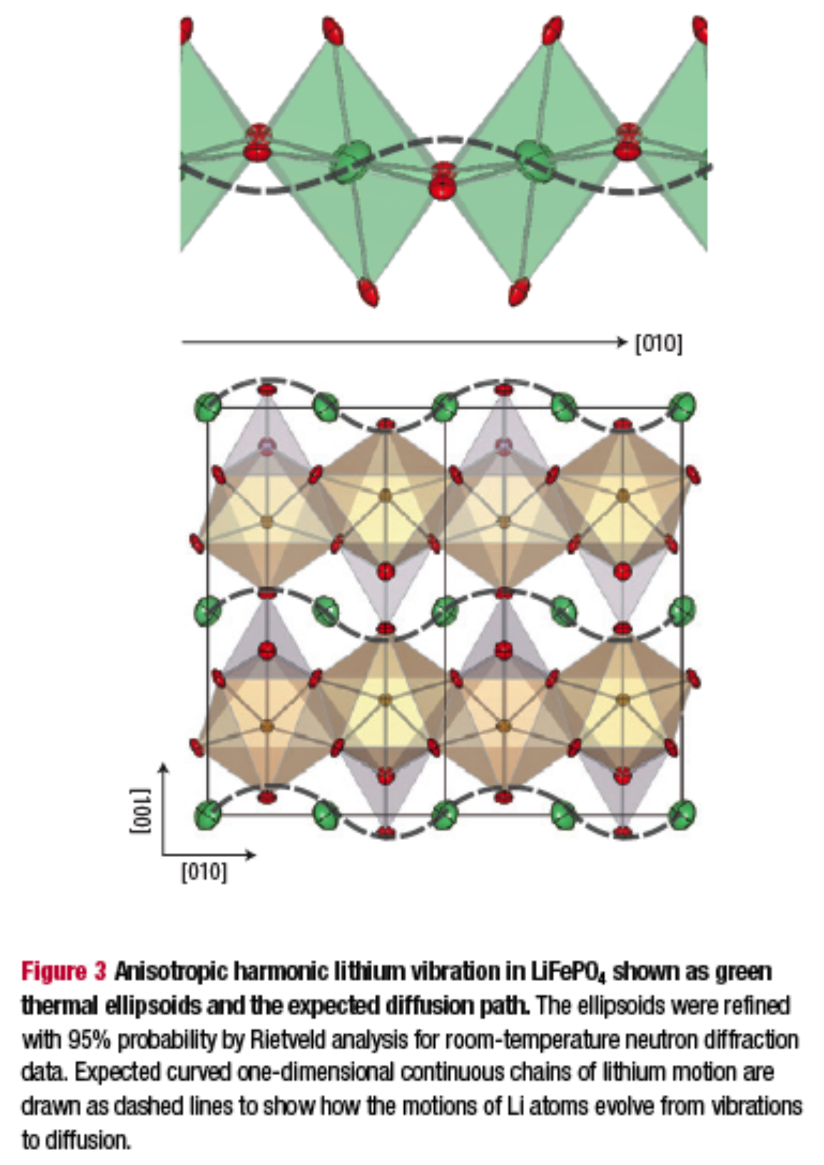
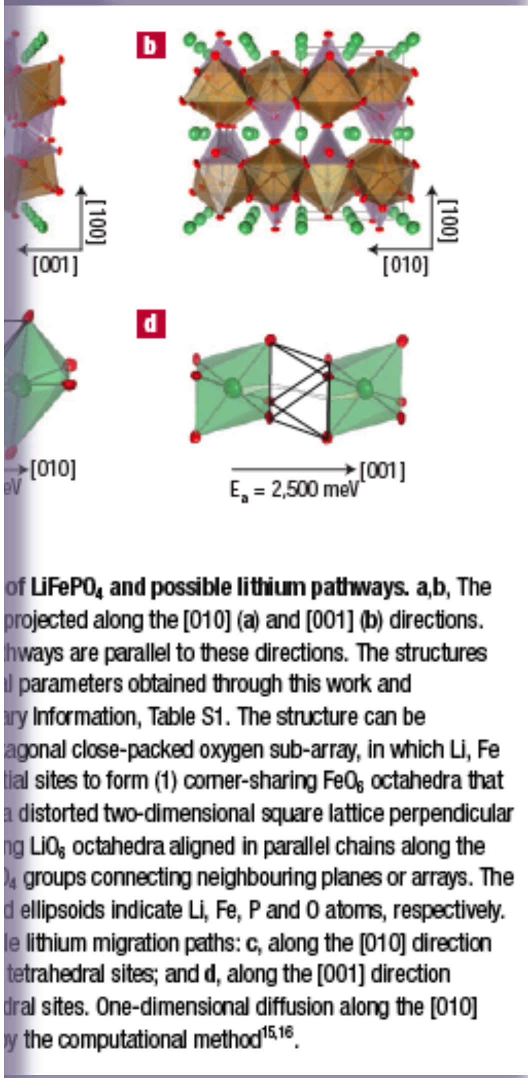


Figure 3 **Anisotropic harmonic lithium vibration in LiFePO$_4$ shown as green thermal ellipsoids and the expected diffusion path.** The ellipsoids were refined with 95% probability by Rietveld analysis for room-temperature neutron diffraction data. Expected curved one-dimensional continuous chains of lithium motion are drawn as dashed lines to show how the motions of Li atoms evolve from vibrations to diffusion.



of LiFePO$_4$ and possible lithium pathways. a,b, The
projected along the [010] (a) and [001] (b) directions.
hways are parallel to these directions. The structures
l parameters obtained through this work and
ry Information, Table S1. The structure can be
agonal close-packed oxygen sub-array, in which Li, Fe
tial sites to form (1) corner-sharing FeO$_6$ octahedra that
a distorted two-dimensional square lattice perpendicular
ng LiO$_6$ octahedra aligned in parallel chains along the
)$_4$ groups connecting neighbouring planes or arrays. The
d ellipsoids indicate Li, Fe, P and O atoms, respectively.
le lithium migration paths: c, along the [010] direction
tetrahedral sites; and d, along the [001] direction
dral sites. One-dimensional diffusion along the [010]
y the computational method[15,16].

EUROPEAN
SPALLATION
SOURCE

Fuel Cells

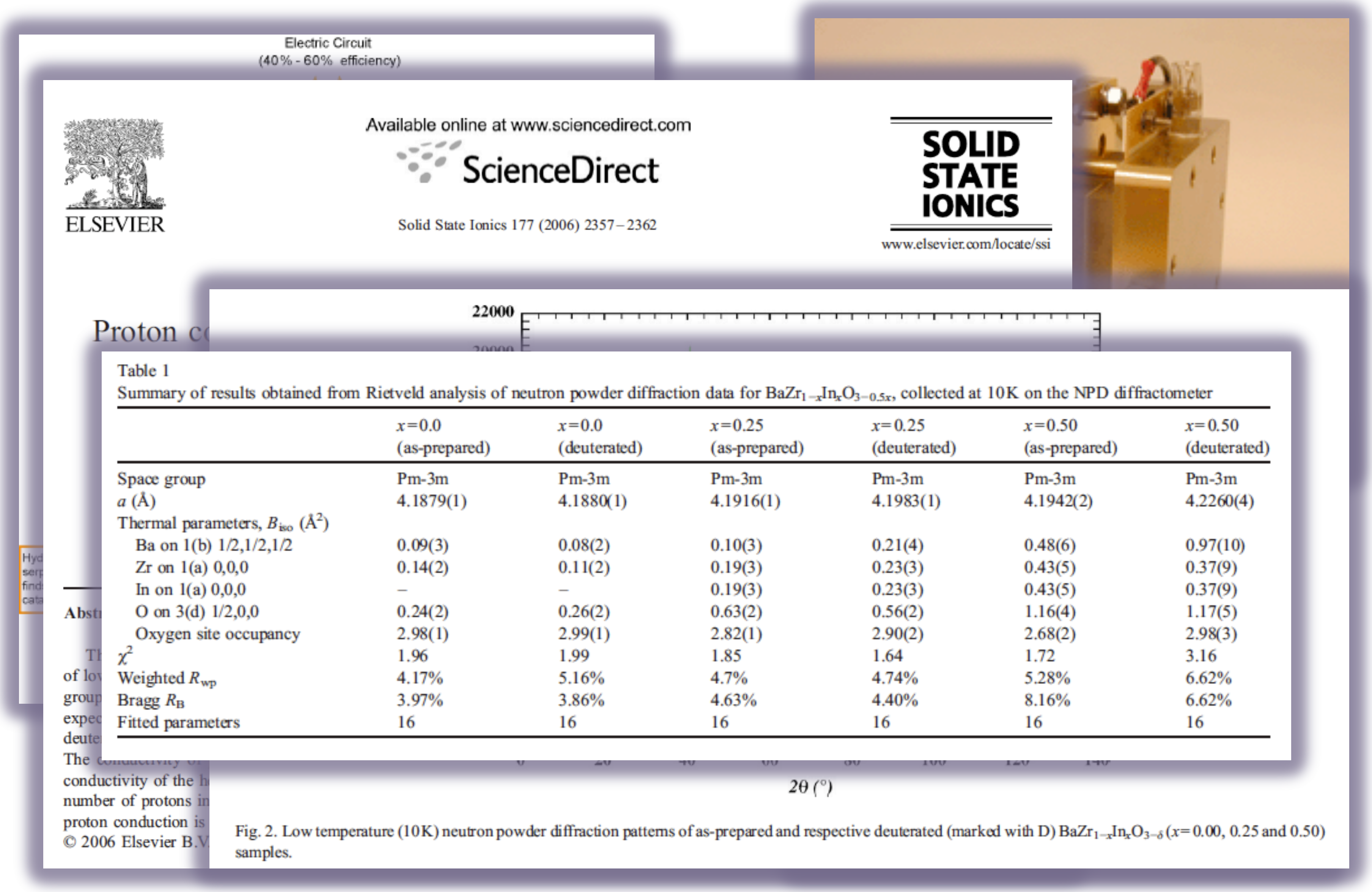


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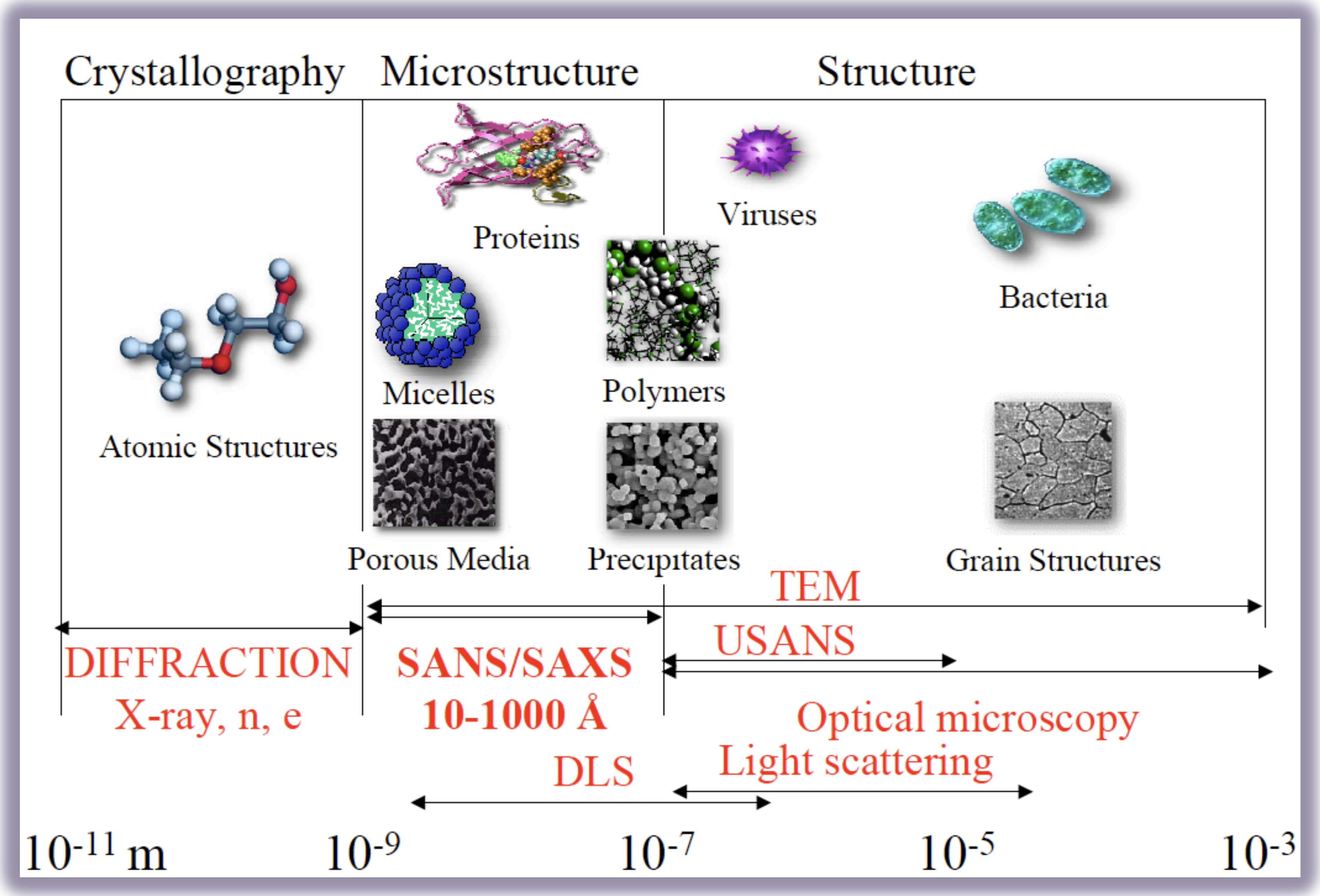
Fig. 2. Low temperature (10K) neutron powder diffraction patterns of as-prepared and respective deuterated (marked with D) $BaZr_{1-x}In_xO_{3-\delta}$ ($x=0.00$, 0.25 and 0.50) samples.

Table 1

Summary of results obtained from Rietveld analysis of neutron powder diffraction data for $BaZr_{1-x}In_xO_{3-0.5x}$, collected at 10K on the NPD diffractometer

	$x=0.0$ (as-prepared)	$x=0.0$ (deuterated)	$x=0.25$ (as-prepared)	$x=0.25$ (deuterated)	$x=0.50$ (as-prepared)	$x=0.50$ (deuterated)
Space group	Pm-3m	Pm-3m	Pm-3m	Pm-3m	Pm-3m	Pm-3m
a (Å)	4.1879(1)	4.1880(1)	4.1916(1)	4.1983(1)	4.1942(2)	4.2260(4)
Thermal parameters, B_{iso} (Å^2)						
Ba on 1(b) 1/2,1/2,1/2	0.09(3)	0.08(2)	0.10(3)	0.21(4)	0.48(6)	0.97(10)
Zr on 1(a) 0,0,0	0.14(2)	0.11(2)	0.19(3)	0.23(3)	0.43(5)	0.37(9)
In on 1(a) 0,0,0	–	–	0.19(3)	0.23(3)	0.43(5)	0.37(9)
O on 3(d) 1/2,0,0	0.24(2)	0.26(2)	0.63(2)	0.56(2)	1.16(4)	1.17(5)
Oxygen site occupancy	2.98(1)	2.99(1)	2.82(1)	2.90(2)	2.68(2)	2.98(3)
χ^2	1.96	1.99	1.85	1.64	1.72	3.16
Weighted R_{wp}	4.17%	5.16%	4.7%	4.74%	5.28%	6.62%
Bragg R_B	3.97%	3.86%	4.63%	4.40%	8.16%	6.62%
Fitted parameters	16	16	16	16	16	16

Small Angle Neutron Scattering



Crystallography

Microstructure

Structure

Proteins

Viruses

Bacteria

Atomic Structures

Micelles

Polymers

Porous Media

Precipitates

Grain Structures

TEM

DIFFRACTION
X-ray, n, e

SANS/SAXS
10-1000 Å

USANS

Optical microscopy

Light scattering

DLS

10^{-11} m

10^{-9}

10^{-7}

10^{-5}

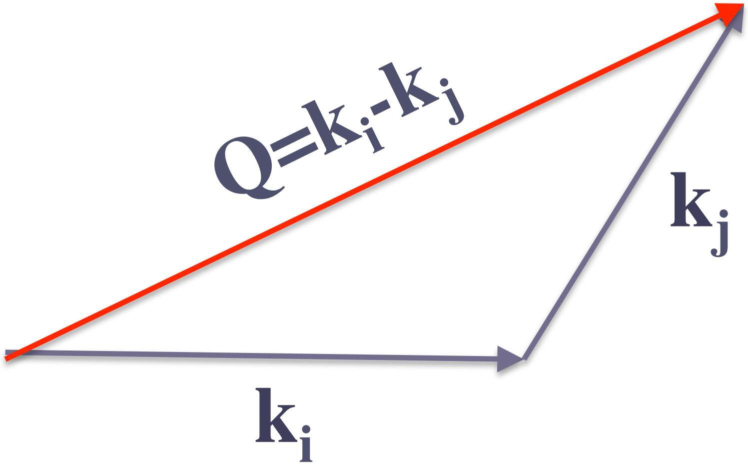
10^{-3}

Small Angle Scattering

- Scattering Vector

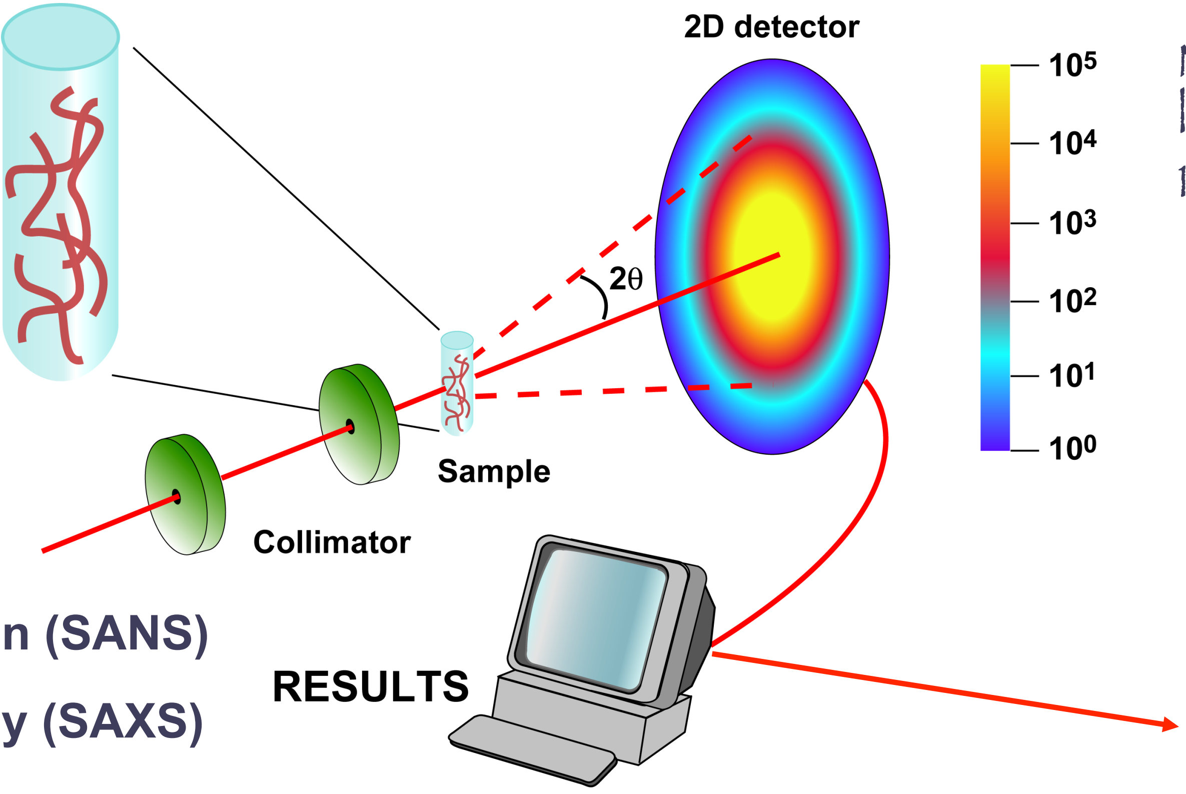
$$\text{Sin } \theta = Q\lambda/4\pi = \lambda/2d$$

$$\rightarrow d = 2\pi/Q$$



Small angle → small Q → large distances
long λ (cold neutrons) ≈ 6 Å, d ≈ 200 Å, $2\theta \approx 1.7°$

SANS: Experimental Setup

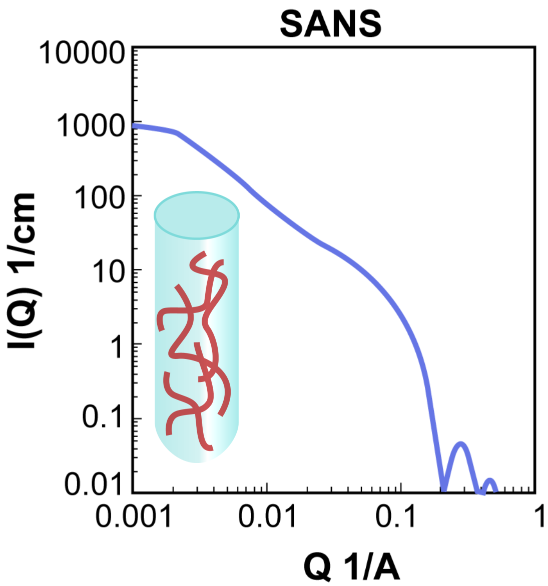


Measures structures at length scales from 1 nm to 100 nm

Beam:

Neutron (SANS)

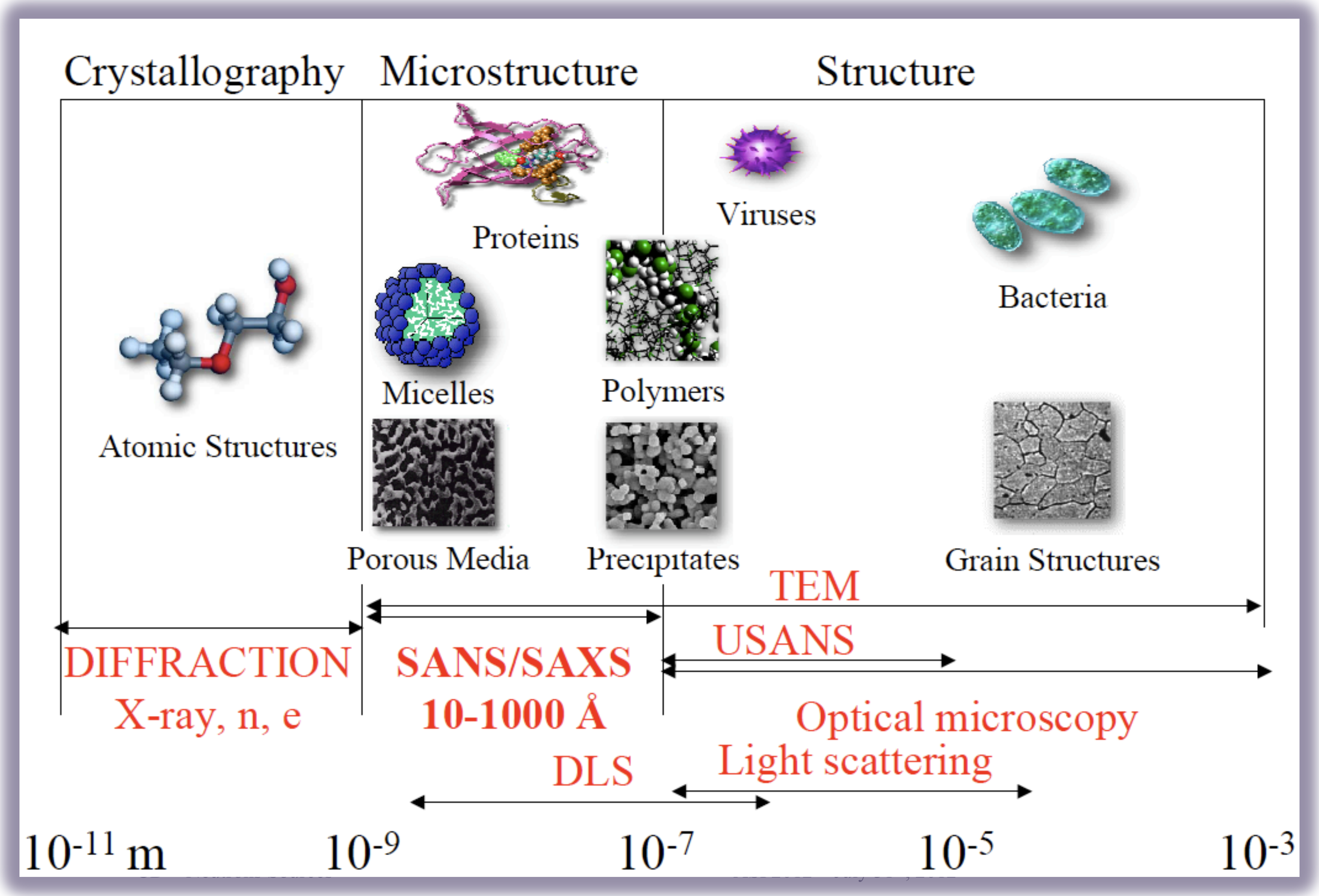
or X-ray (SAXS)



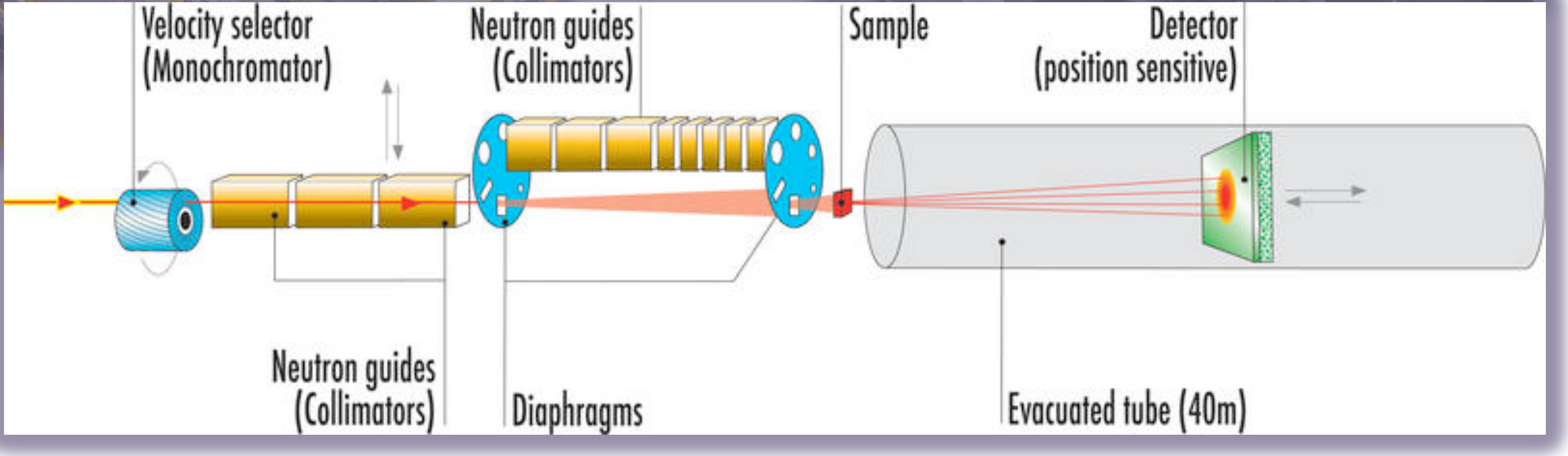
$$|Q| = \frac{4\pi \sin\theta}{\lambda}$$

$$\boxed{\Theta_{min} \approx 0.03°, \ \Theta_{max} \approx 3°}$$

SANS: applications



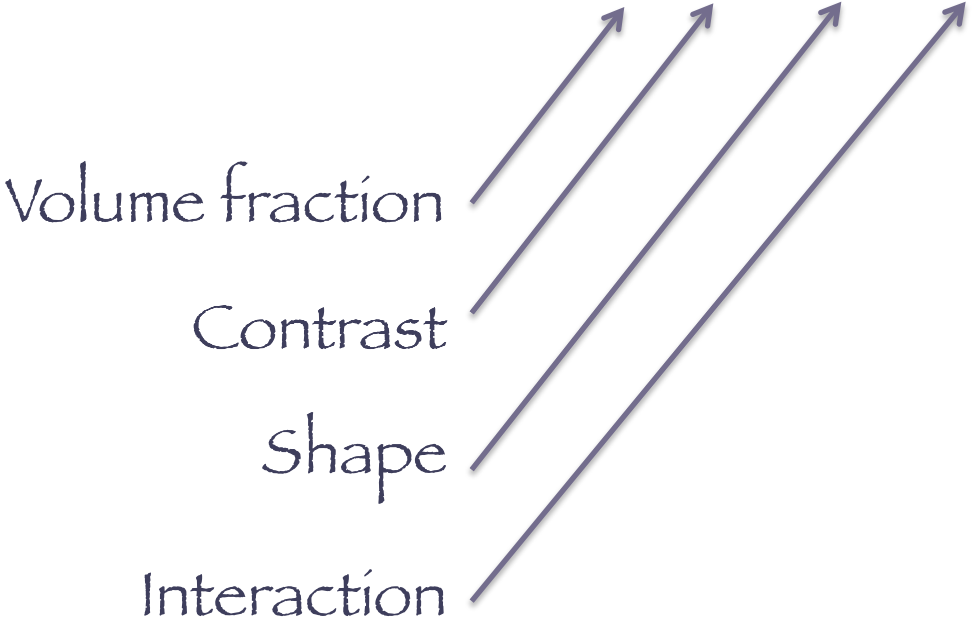
Small Angle Instruments



Scattering

- **Cross section:** $d\sigma = \dfrac{(\#\ \text{particles scattered into solid angle } \Delta\Omega/\text{s})}{(\#\ \text{particles incident/sec})(\#\ \text{scattering centers/area})}$

$$\frac{d\sigma(Q)}{d\Omega} = N_p V_p \overline{\rho} P(Q) S(Q)$$



Volume fraction

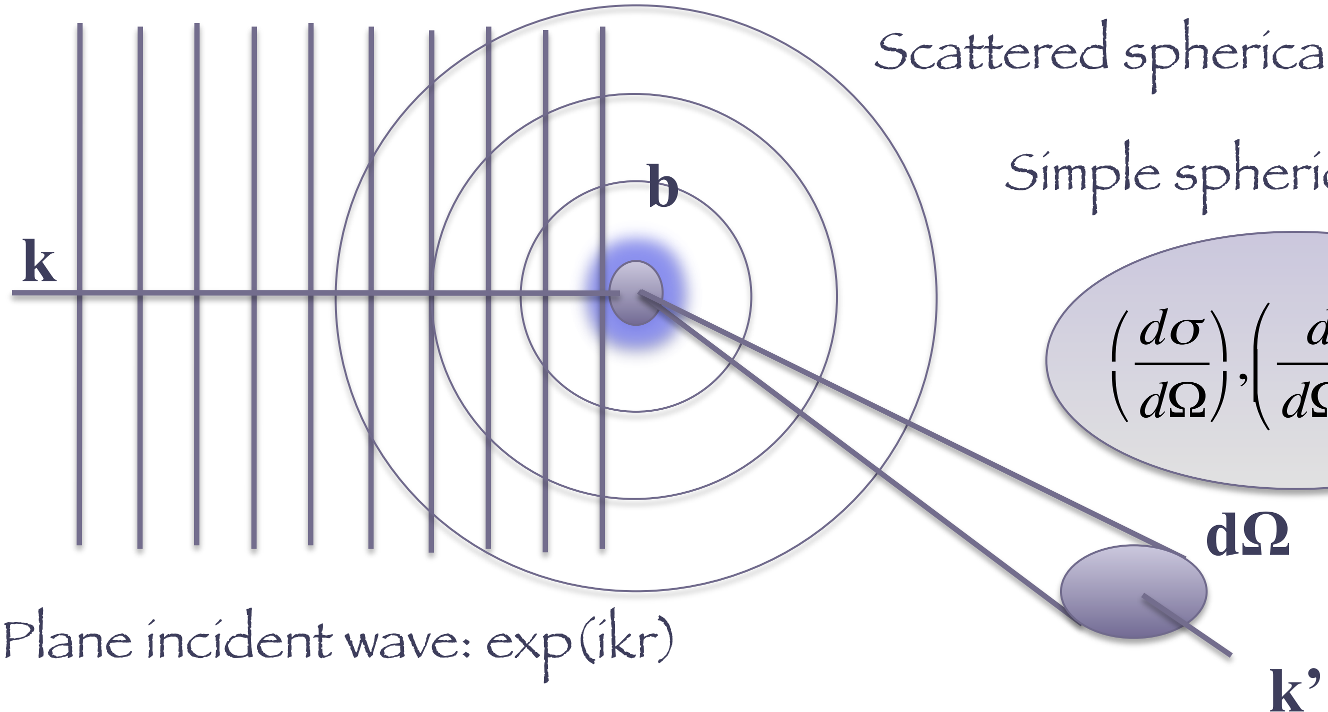
Contrast

Shape

Interaction

SANS: Scattering of plane wave

σ_{tot}=number of neutrons scattered in all directions per sec/incident flux



Scattered spherical wave: –b exp(ikr)/b

Simple spherical object!!

$$\left(\frac{d\sigma}{d\Omega}\right),\left(\frac{d^2\sigma}{d\Omega\, dE}\right)$$

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

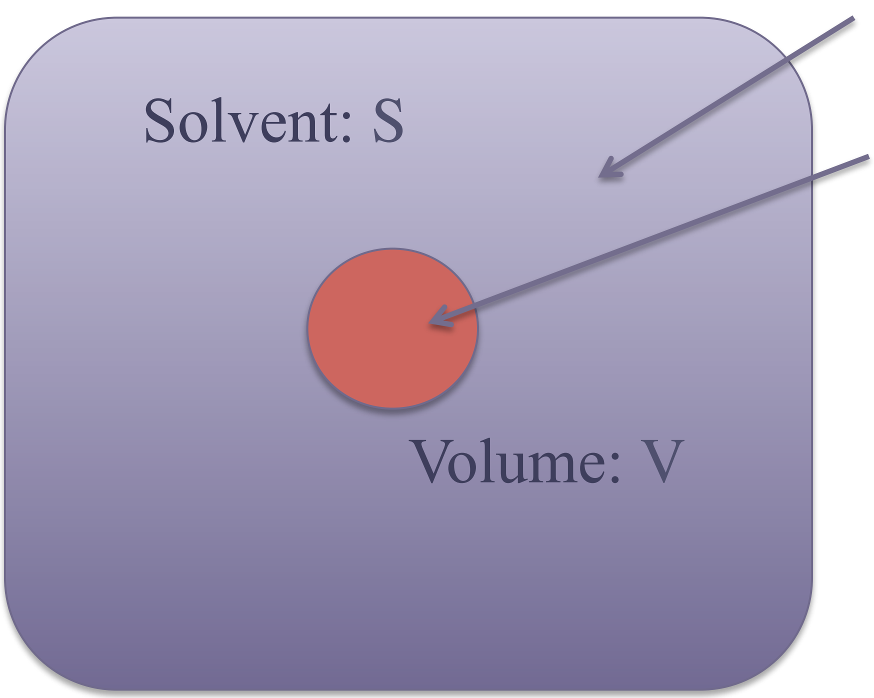
Plane incident wave: exp(ikr)

$$\frac{d\sigma(Q)}{d\Omega} = N_p V_p \overline{\rho} P(Q) S(Q)$$

Volume fraction

Contrast

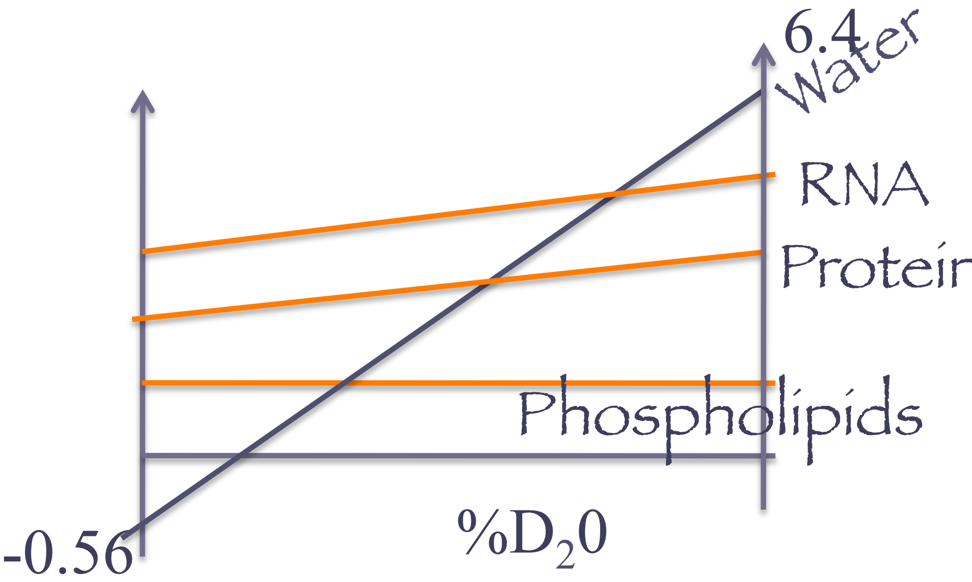
SANS: Particles: contrast!



Density: ρ_S

Density: ρ_V

Contrast! $\overline{\rho}_p = \rho_V - \rho_S$

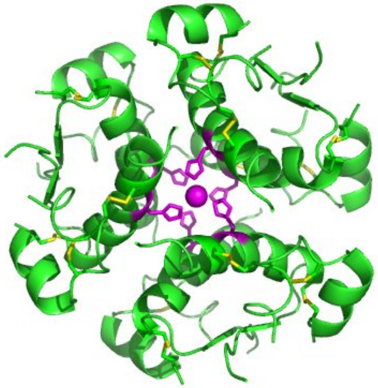


SANS: quick example

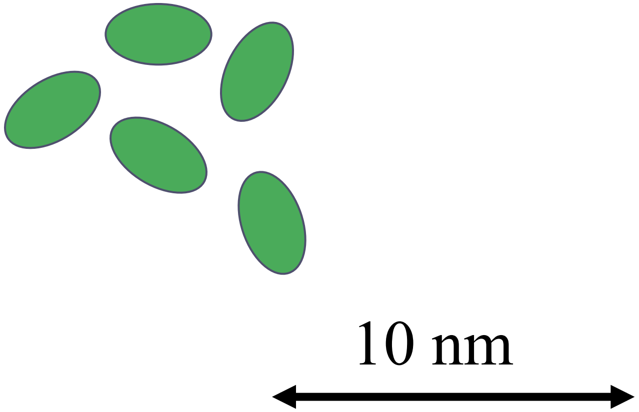
Protein based drugs:

- Typically proteins in solution to be injected
- Long shelf life (up to 2 years)
- Control of release profile is desirable

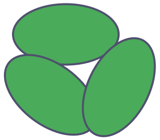
Insulin Hexamer



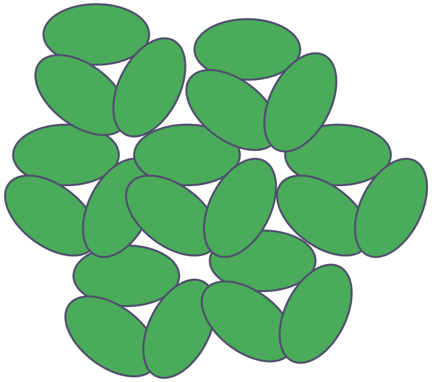
Fast action: Monomeric and dimeric insulin



Medium action: Hexameric insulin



Slow action: Large complexes of hexameric insulin

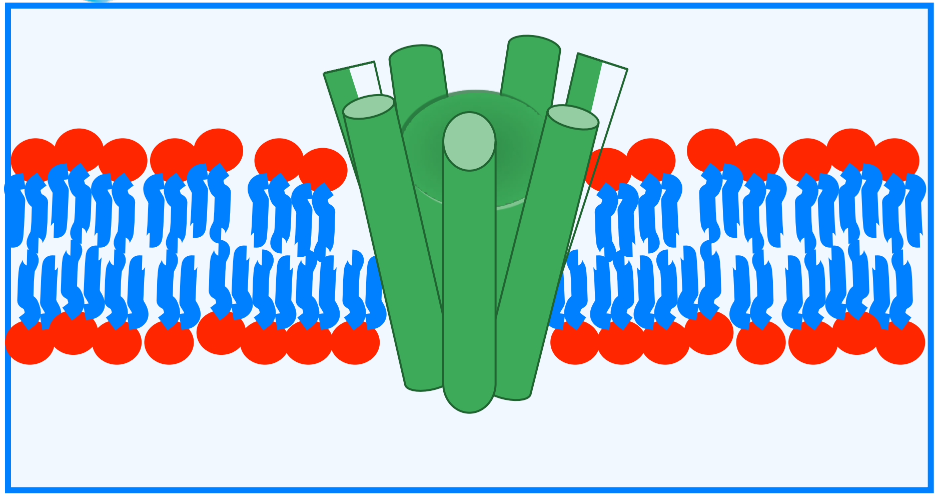


Knowledge and control of solution properties of the proteins are crucial

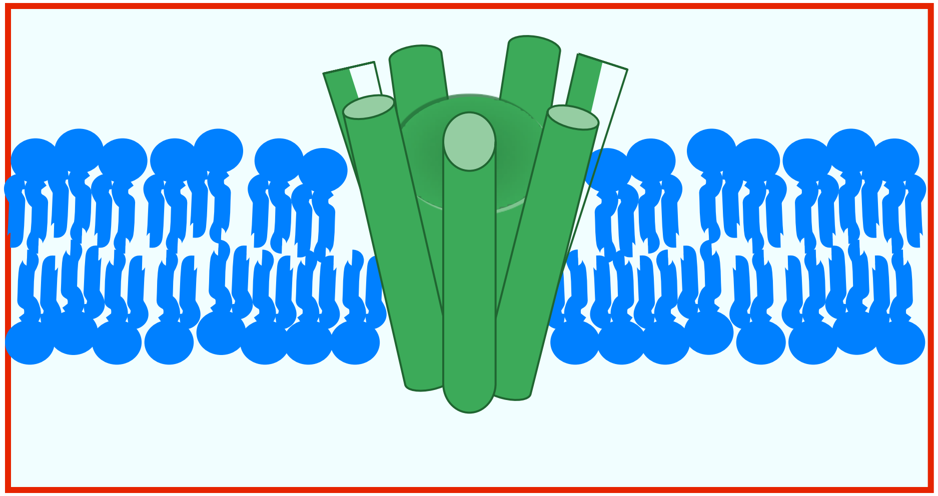
Source: L Arleth, Uni Copenhagen

SANS versus SAXS

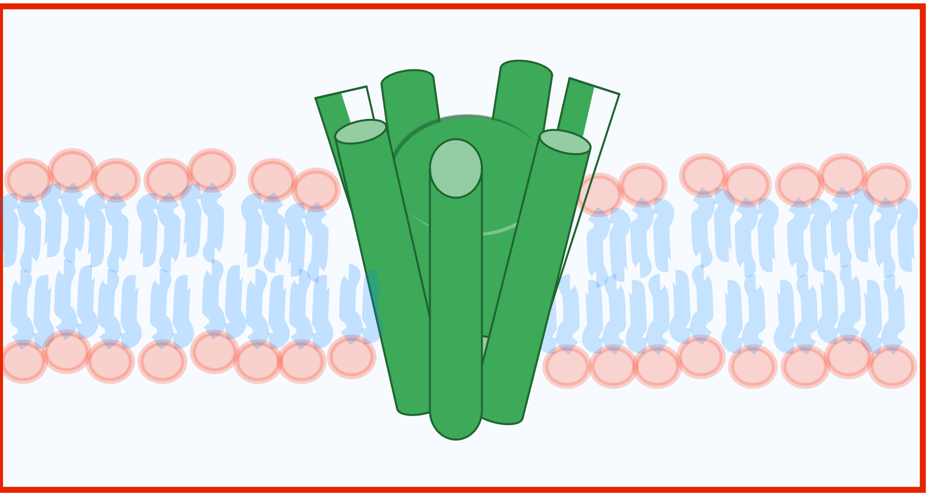
SAXS contrast



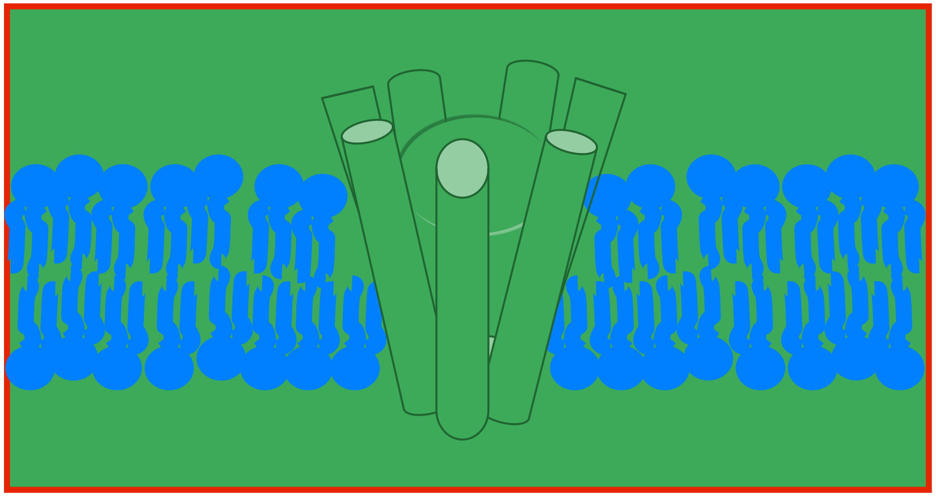
SANS contrast 1



SANS contrast 2



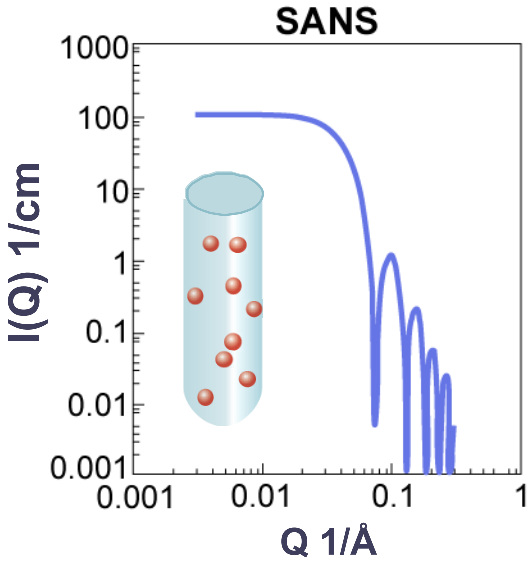
SANS contrast 3



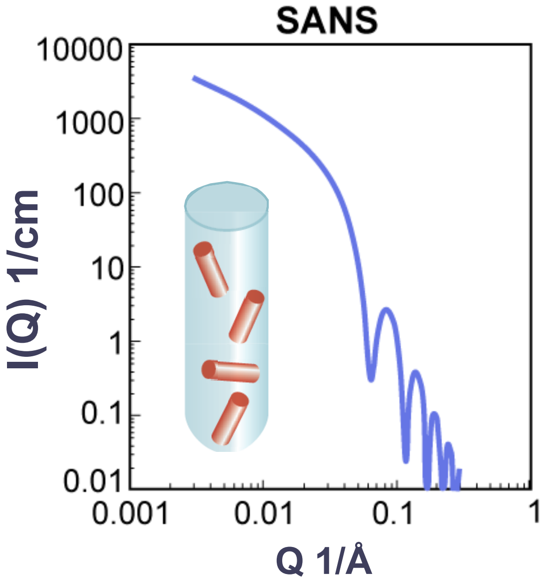
SANS gives the possibility of **not** seing everything at the same time….

SANS: Different Shapes

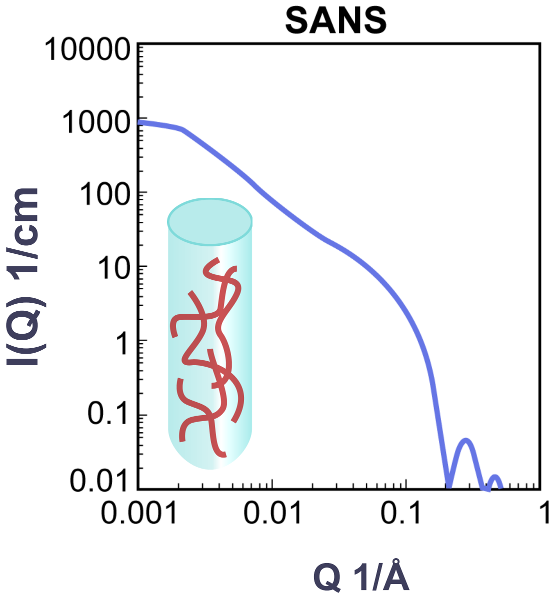
- **Spheres:**
  R = 60 Å



Rods: R = 60 Å
L = 1200 Å

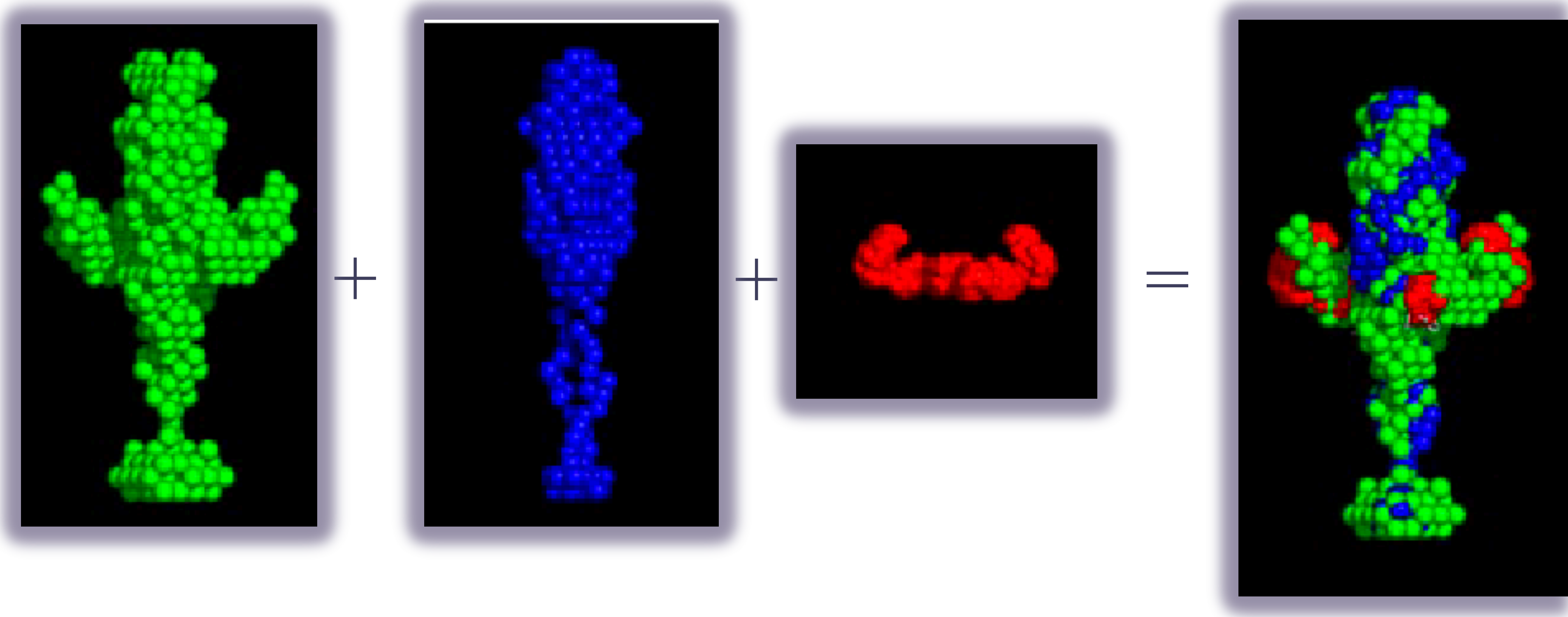


Worms: R = 18 Å
L = 5000 Å,
Kuhn Length = 300 Å



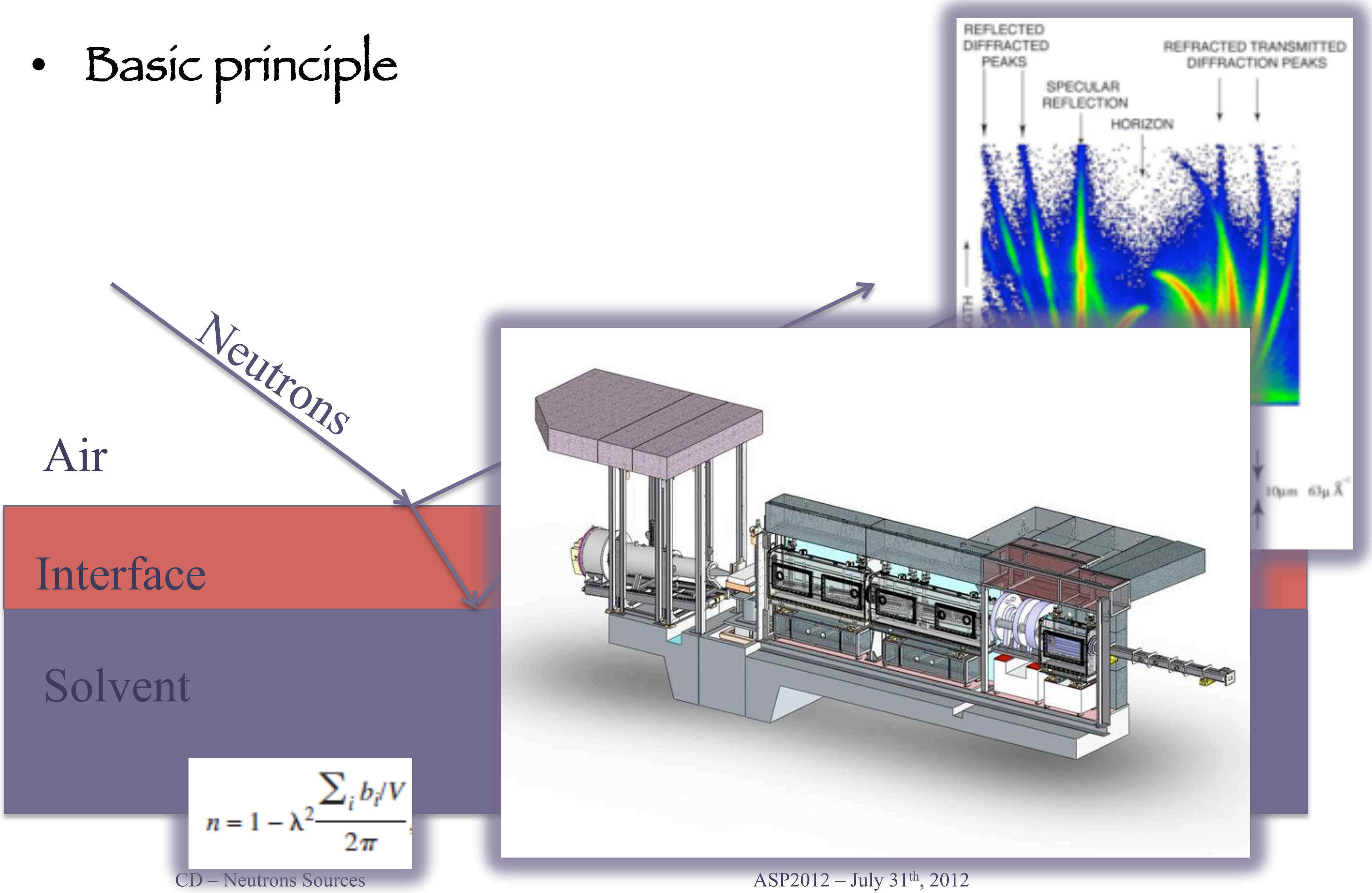
SANS: Selective Deuteration

sensitivity and selectivity
isotopic substitution/contrast variation



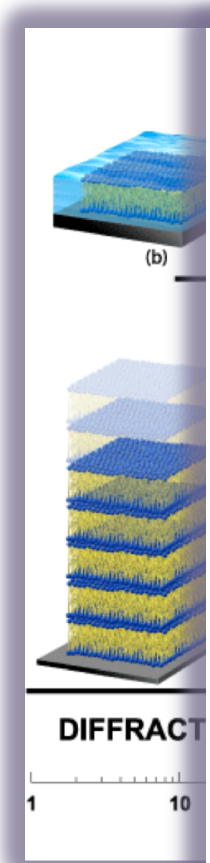
Neutron Reflectivity

- Basic principle



$$n = 1 - \lambda^2 \frac{\sum_i b_i/V}{2\pi}$$

Neutron Reflectivity



Neutron reflectometry to investigate the delivery of lipids and DNA to interfaces (Review)

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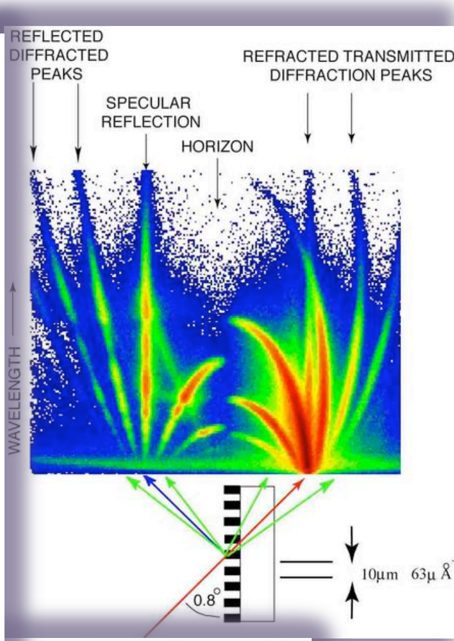
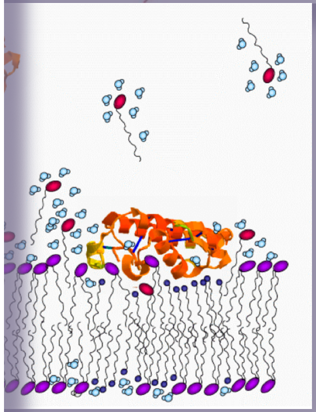
The application of scattering methods in the study of biological and biomedical problems is a field of research that is currently experiencing fast growth. In particular, neutron reflectometry (NR) is a technique that is becoming progressively more widespread, as indicated by the current commissioning of several new reflectometers worldwide. NR is valuable for the characterization of biomolecules at interfaces due to its capability to provide quantitative structural and compositional information on relevant molecular length scales. Recent years have seen an increasing number of applications of NR to problems related to drug and gene delivery. We start our review by summarizing the experimental methodology of the technique with reference to the description of biological liquid interfaces. Various methods for the interpretation of data are then discussed, including a new approach based on the lattice mean-field theory to help characterize stimulus-responsive surfaces relevant to drug delivery function. Recent progress in the subject area is reviewed in terms of NR studies relevant to the delivery of lipids and DNA to surfaces. Lastly, we discuss two case studies to exemplify practical features of NR that are exploited in combination with complementary techniques. The first case concerns the interactions of lipid-based cubic phase nanoparticles with model membranes (a drug delivery application), and the second case concerns DNA compaction at surfaces and in the bulk solution (a gene delivery application). © *2008 American Vacuum Society.* [DOI: 10.1116/1.2976448]





Fission and Spallation

FISSION

Courtesy of Konstantin Batkov

Example

$$n + {}^{235}U \longrightarrow {}^{95}Sr + {}^{139}Xe + 2n$$

Why incident neutron?

- Zero electric charge ($\Rightarrow$ no Coulomb's repulsion) allows the neutrons of very low energy to approach the nucleus at $l \ll L_{nucl}$
- Very high fission cross-section with ${}^{235}U$.

Why ${}^{235}U$?

- Most of heavy nuclei can undergo the fission reaction initiated by neutrons, but ${}^{235}U$ has very high cross section with thermal neutrons.
- No fission threshold energy $\Rightarrow$ incident neutrons can be very slow.

Prompt neutrons

- Average energy: $\sim 1\,\text{MeV}$

Fission fragments

- Beta radioactive

➔ Chain Reaction

The spallation process

Spallation Neutron Yield (i.e. multiplicity of emitted neutrons)

determines the requirement in terms of the accelerator power (current and energy of incident proton beam).

Spallation Neutron Spectrum (i.e. energy distribution of emitted neutrons)

determines the damage and activation of the structural materials (design of the beam window and spallation target)

Spallation Product Distributions

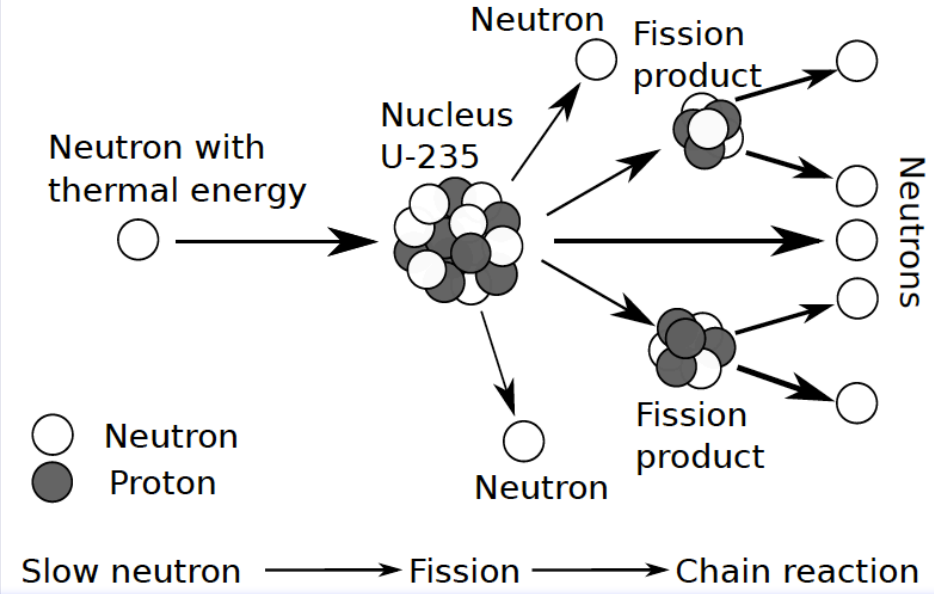
determines the radiotoxicity of the residues (radioprotection requirements).

Energy Deposition

determines the thermal-hydraulic requirements (cooling capabilities and nature of the spallation target).

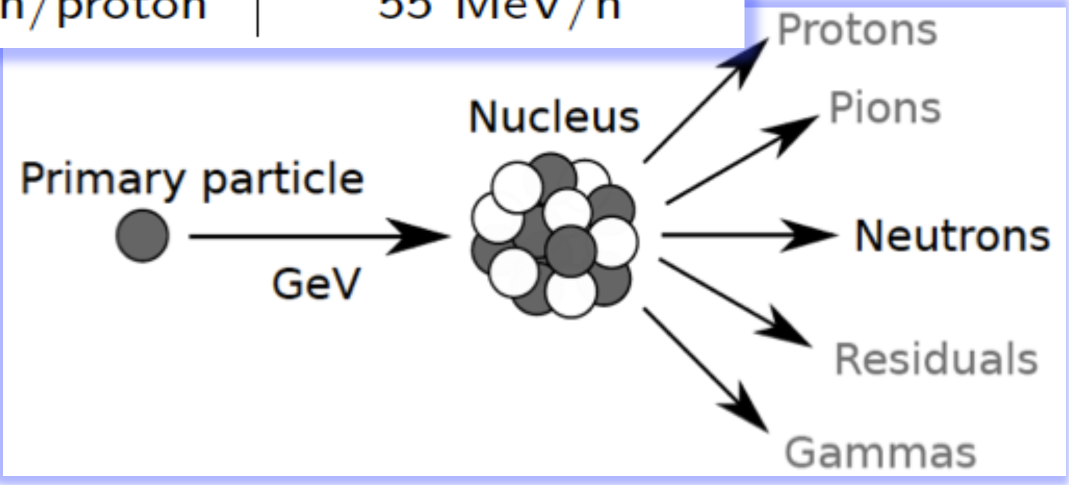
➔ **Sub-critical Reaction**

Fission and Spallation

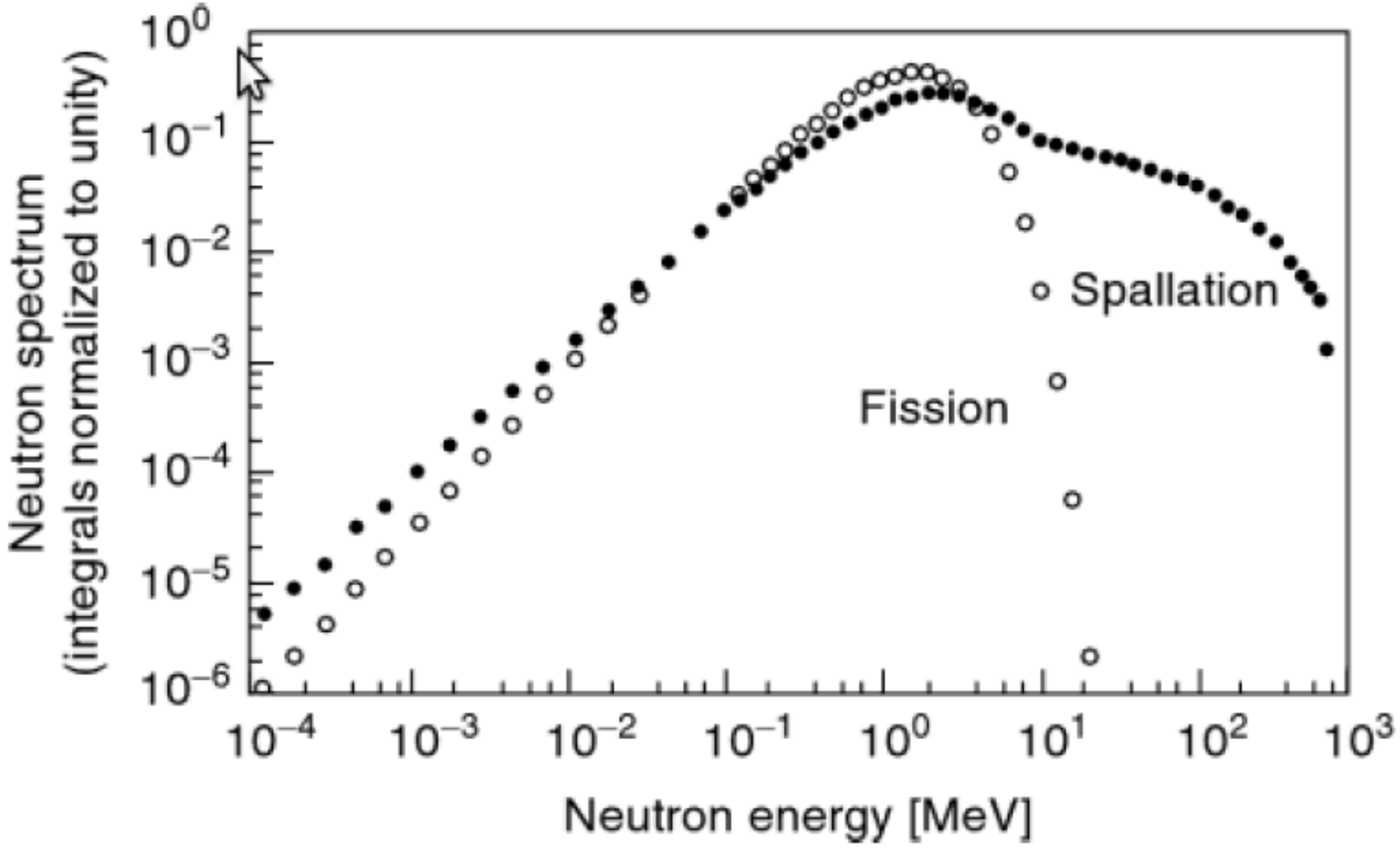


Spallation is a non-elastic nuclear interaction induced by a high-energy particle producing numerous secondary particles

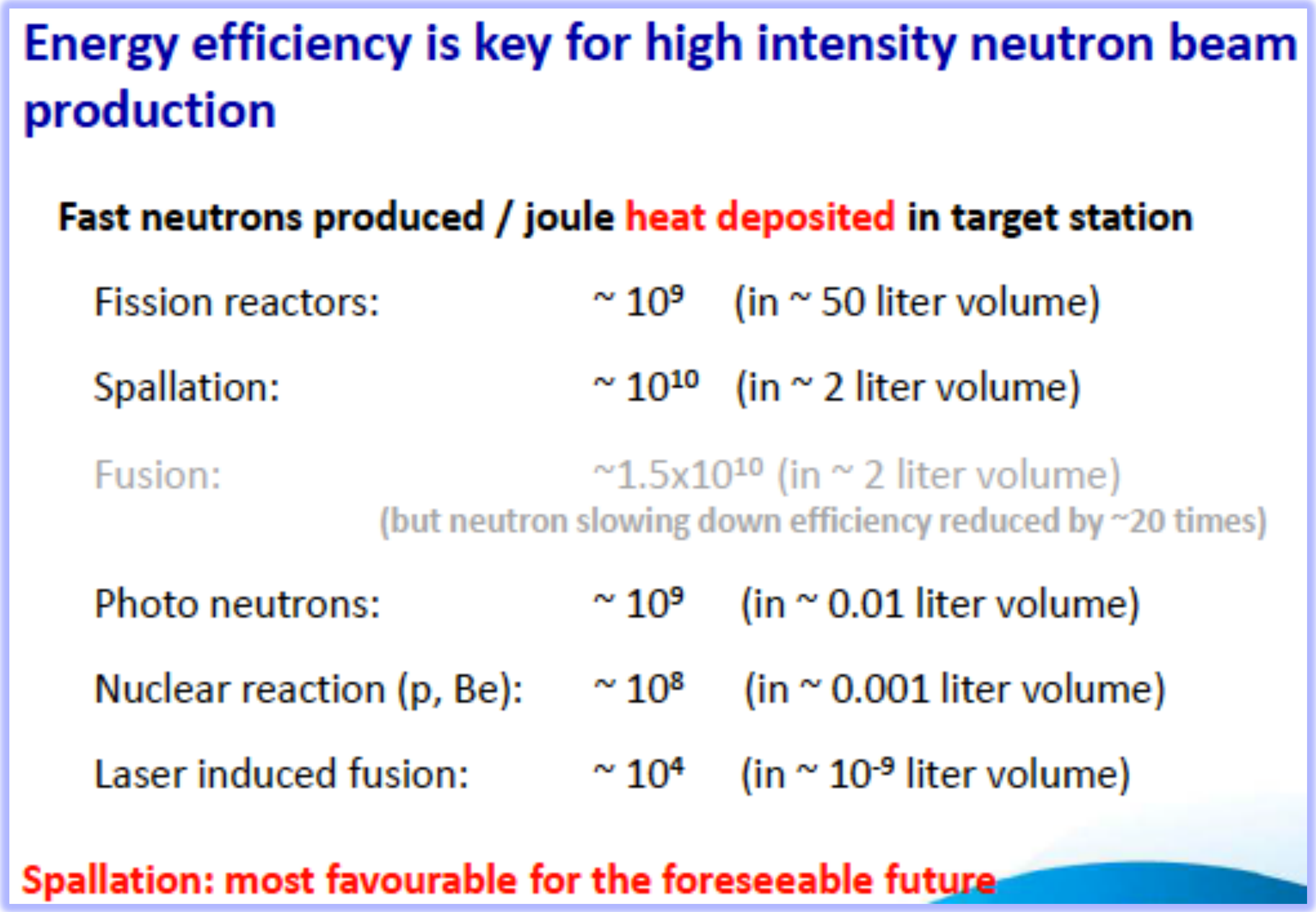
Process	Reaction	Neutron yield	Energy deposition
Fission	^{235}U(n,f)	3 n/fission	190 MeV/n
Spallation	p 1 GeV $\rightarrow$ Hg	30 n/proton	55 MeV/n



Fission and Spallation



[D. Filges and F. Goldenbaum, Handbook of Spallation Research]



Energy efficiency is key for high intensity neutron beam production

Fast neutrons produced / joule heat deposited in target station

Fission reactors:	~ 10^9	(in ~ 50 liter volume)
Spallation:	~ 10^{10}	(in ~ 2 liter volume)
Fusion:	~$1.5x10^{10}$	(in ~ 2 liter volume) (but neutron slowing down efficiency reduced by ~20 times)
Photo neutrons:	~ 10^9	(in ~ 0.01 liter volume)
Nuclear reaction (p, Be):	~ 10^8	(in ~ 0.001 liter volume)
Laser induced fusion:	~ 10^4	(in ~ 10^{-9} liter volume)

Spallation: most favourable for the foreseeable future