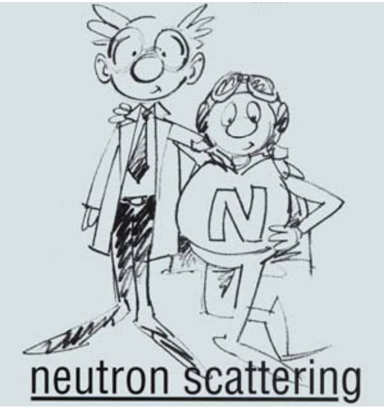

Methods and Concepts of Neutron scattering

by

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Outline

- What do we try to measure with neutron scattering?
    - Introduction to nuclear and magnetic neutron scattering
    - Elastic and inelastic scattering
    - Coherent and incoherent scattering
    - Introduction to correlation functions in space and time
    - Real space and reciprocal space

- How do we make the measurement?
    - Scattering triangles and kinematic constraints
    - CW and TOF approaches
    - Review of some typical neutron scattering instruments
    - Why are there so many different types of neutron instrument?

- What are the obstacles?

Why do Neutron Scattering?

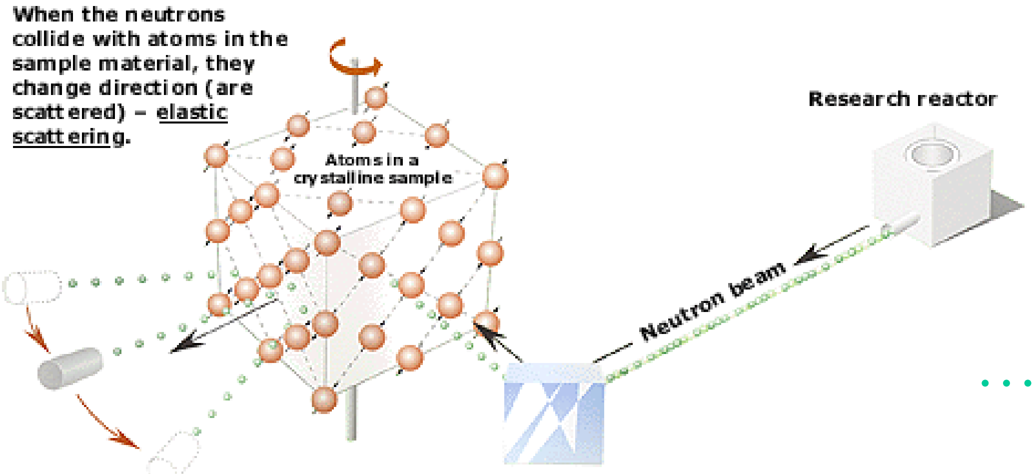
- To determine the positions and motions of atoms in condensed matter
  - 1994 Nobel Prize to Shull and Brockhouse cited these areas

- Neutron advantages:
  - Wavelength comparable with interatomic spacings
  - Kinetic energy comparable with that of atoms in a solid
  - Penetrating => bulk properties are measured & sample can be contained
  - Weak interaction with matter aids interpretation of scattering data
  - Isotopic sensitivity allows contrast variation
  - Neutron magnetic moment couples to ***B*** => neutron “sees” unpaired electron spins

- Neutron Disadvantages
  - Neutron sources are weak => low signals, need for large samples etc
  - Some elements (e.g. Cd, B, Gd) absorb strongly
  - Kinematic restrictions (can’t access all energy & momentum transfers)

The 1994 Nobel Prize in Physics – Shull & Brockhouse

Neutrons show where the atoms are….

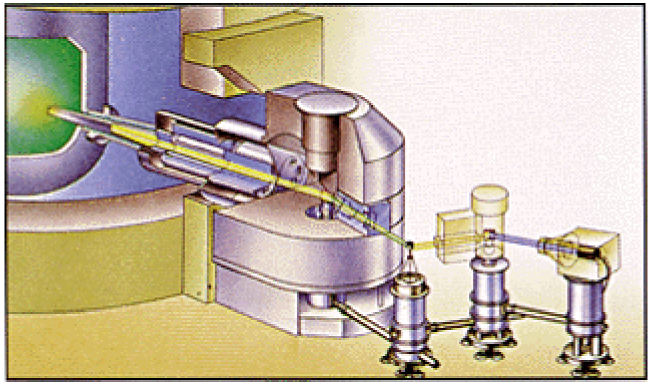


When the neutrons collide with atoms in the sample material, they change direction (are scattered) – elastic scattering.

Detectors record the directions of the neutrons and a diffraction pattern is obtained.

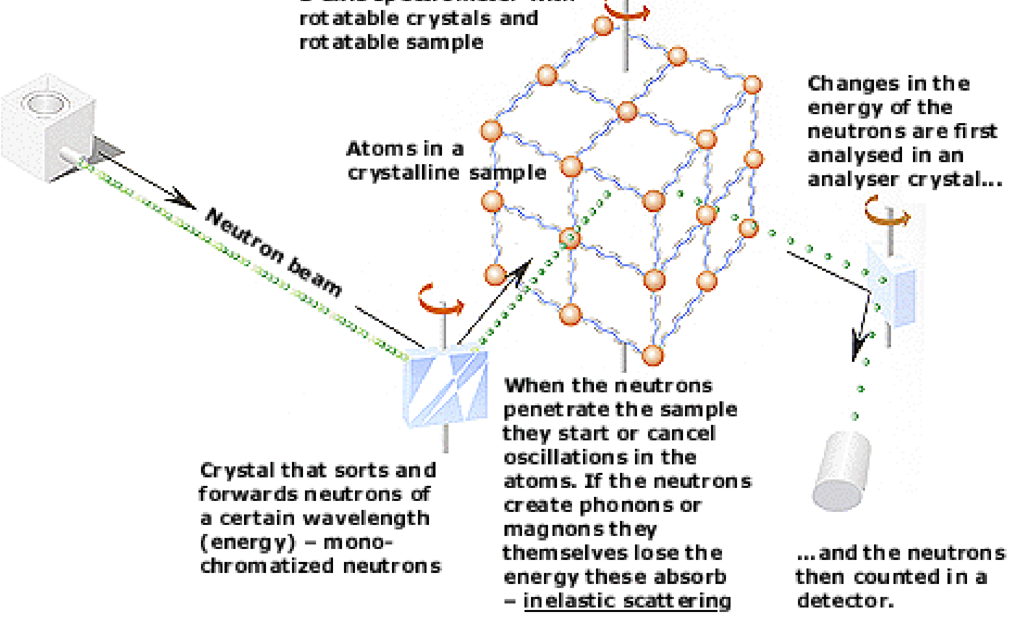
The pattern shows the positions of the atoms relative to one another.

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



3-axis spectrometer

…and what the 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.

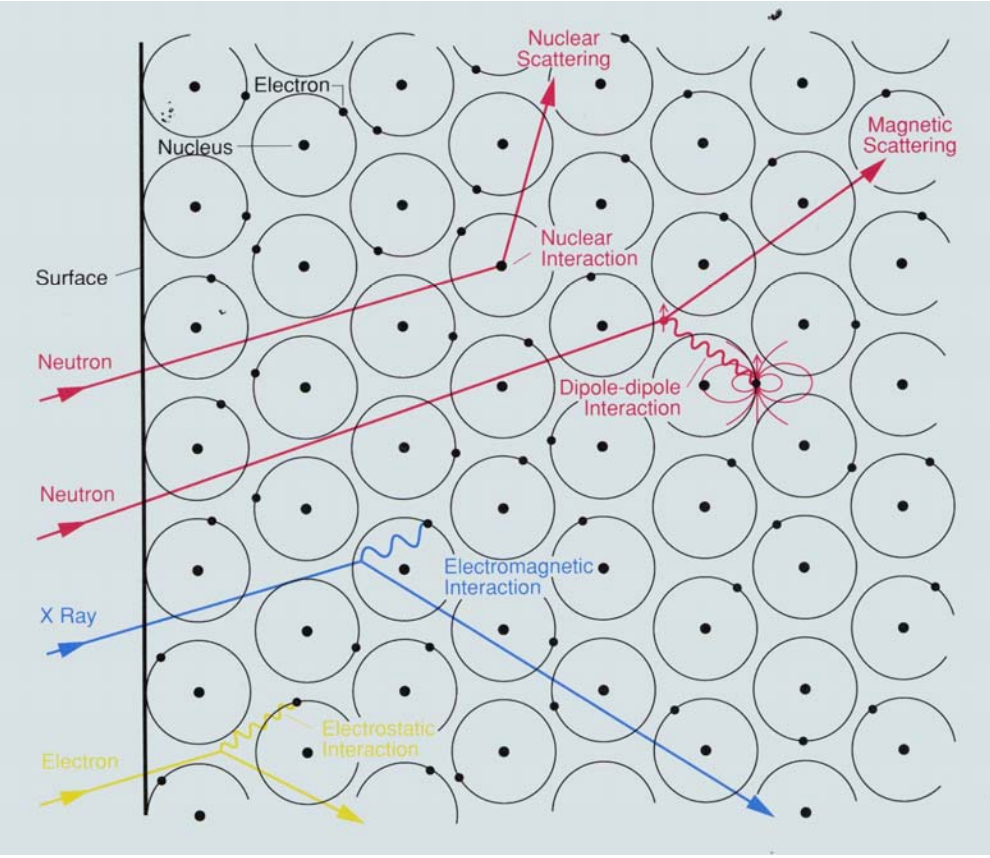
Historical accomplishments of Neutron Scattering

- Antiferromagnetic Structures
- Rare earth spirals and other spin structures
- Spin wave dispersion
- Our whole understanding of the details of exchange interactions in solids
- Magnetism and Superconductivity
- Phonon dispersion curves in crystals; quantum crystals and anharmonicity
- Crystal fields
- Excitations in normal liquids
- Rotons in superfluid helium
- Condensate fraction in helium

More Recent Applications of Neutrons

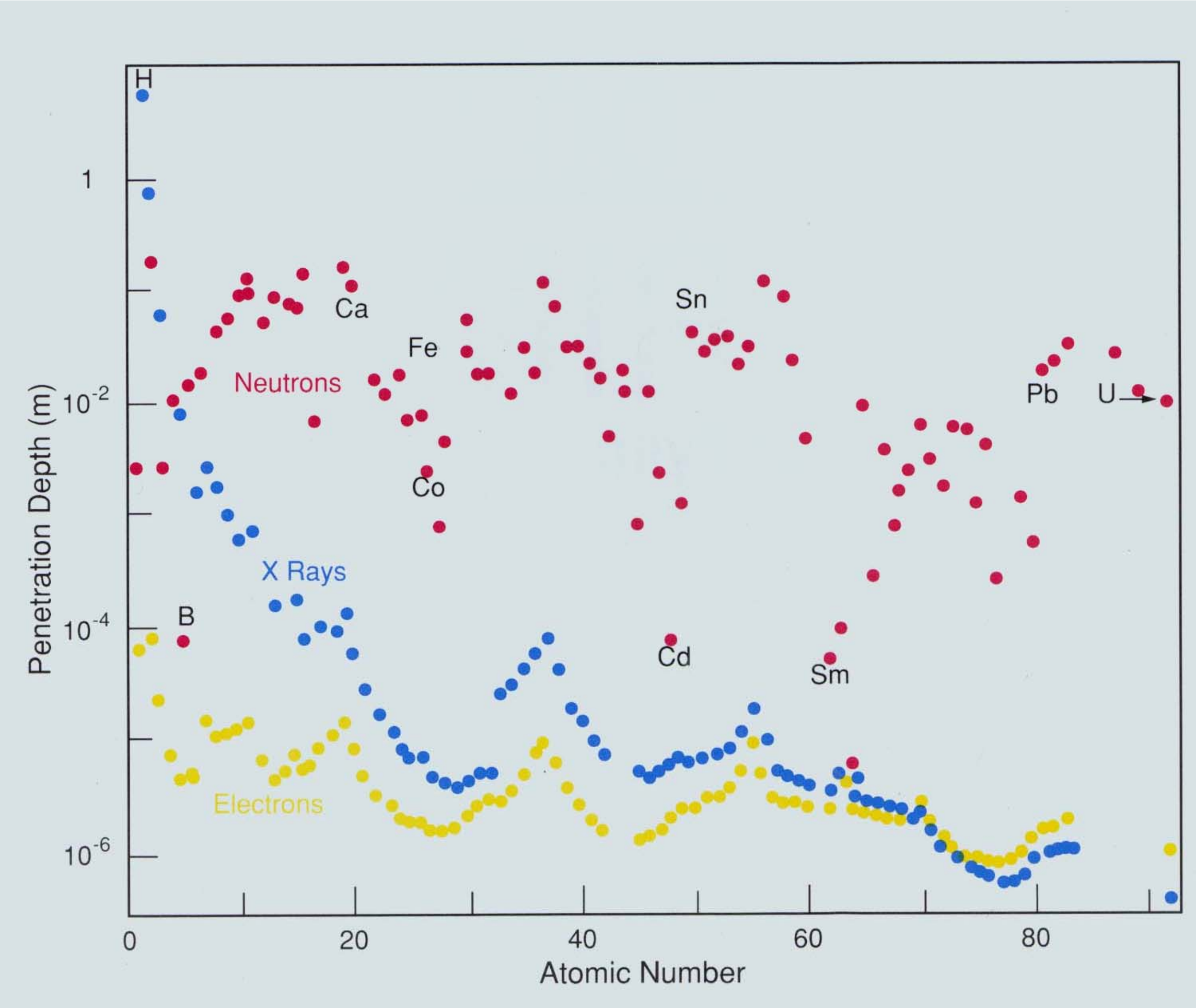
- Quantum Phase Transitions and Critical points
- Magnetic order and magnetic fluctuations in the high-Tc cuprates
- Gaps and low-lying excitations (including phonons) in High-Tc
- Magnetic Order and spin fluctuations in highly-correlated systems
- Manganites
- Magntic nanodot/antidot arrays
- Exchange bias
- Proton motion in carbon nanotubes
- Protein dynamics
- Glass transition in polymer films
- Protonation states in biological macromolecules from nuclear density maps
- Studies of protein diffusive motion in hydrated enzymes

Interaction Mechanisms



- Neutrons interact with atomic nuclei via very short range (~fm) forces.
- Neutrons interact with unpaired electrons via magnetic dipole interaction.
- X-rays interact with electrons via an electromagnetic interaction

Thermal Neutrons, 8 keV X-Rays & Low Energy Electrons:- Penetration in Matter



Note for neutrons:

- H/D difference
- Cd, B, Sm
- no systematic Z dependence

For x-rays:

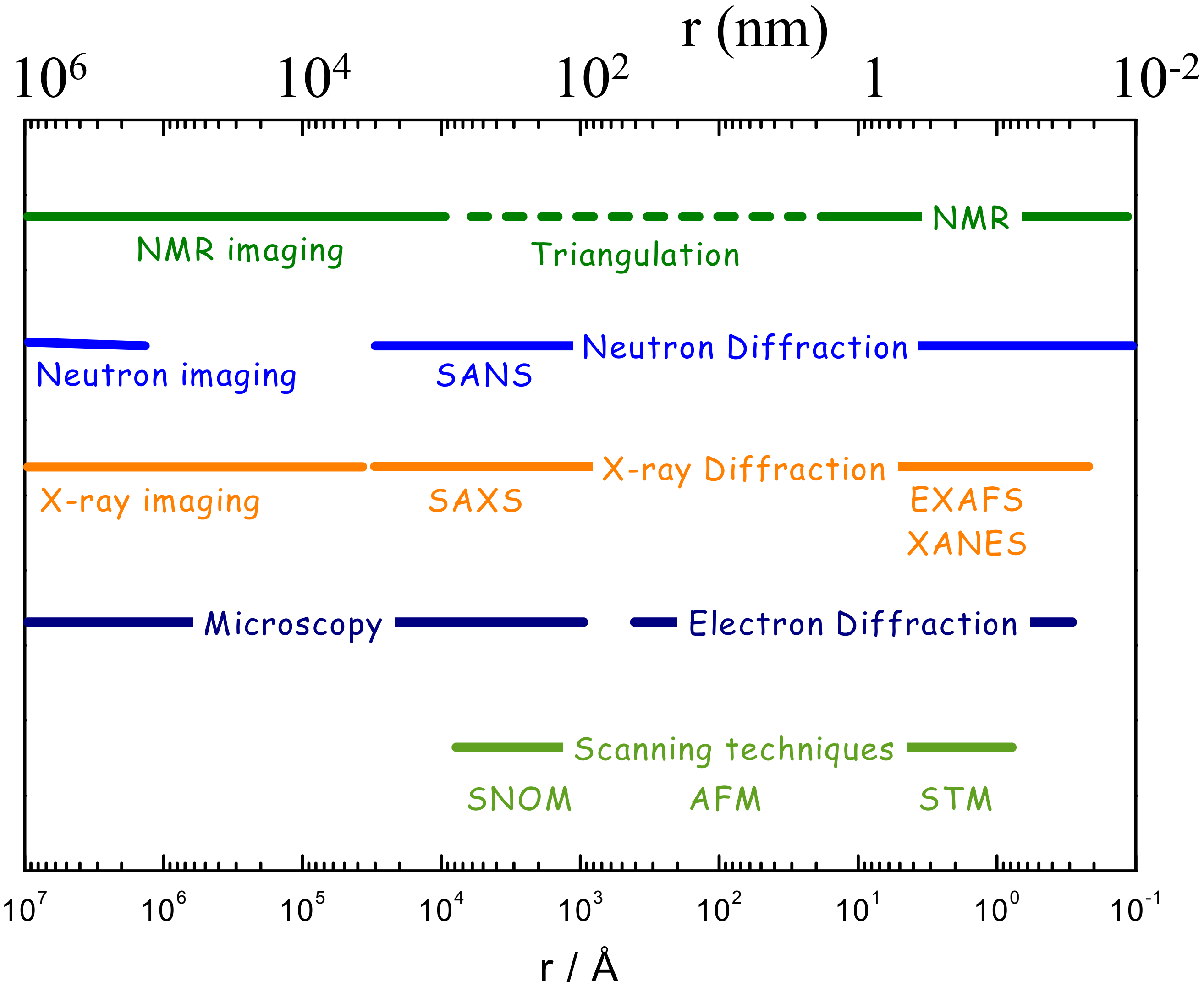
- decreasing penetration as Z increases

Types of Neutron-Material Interactions

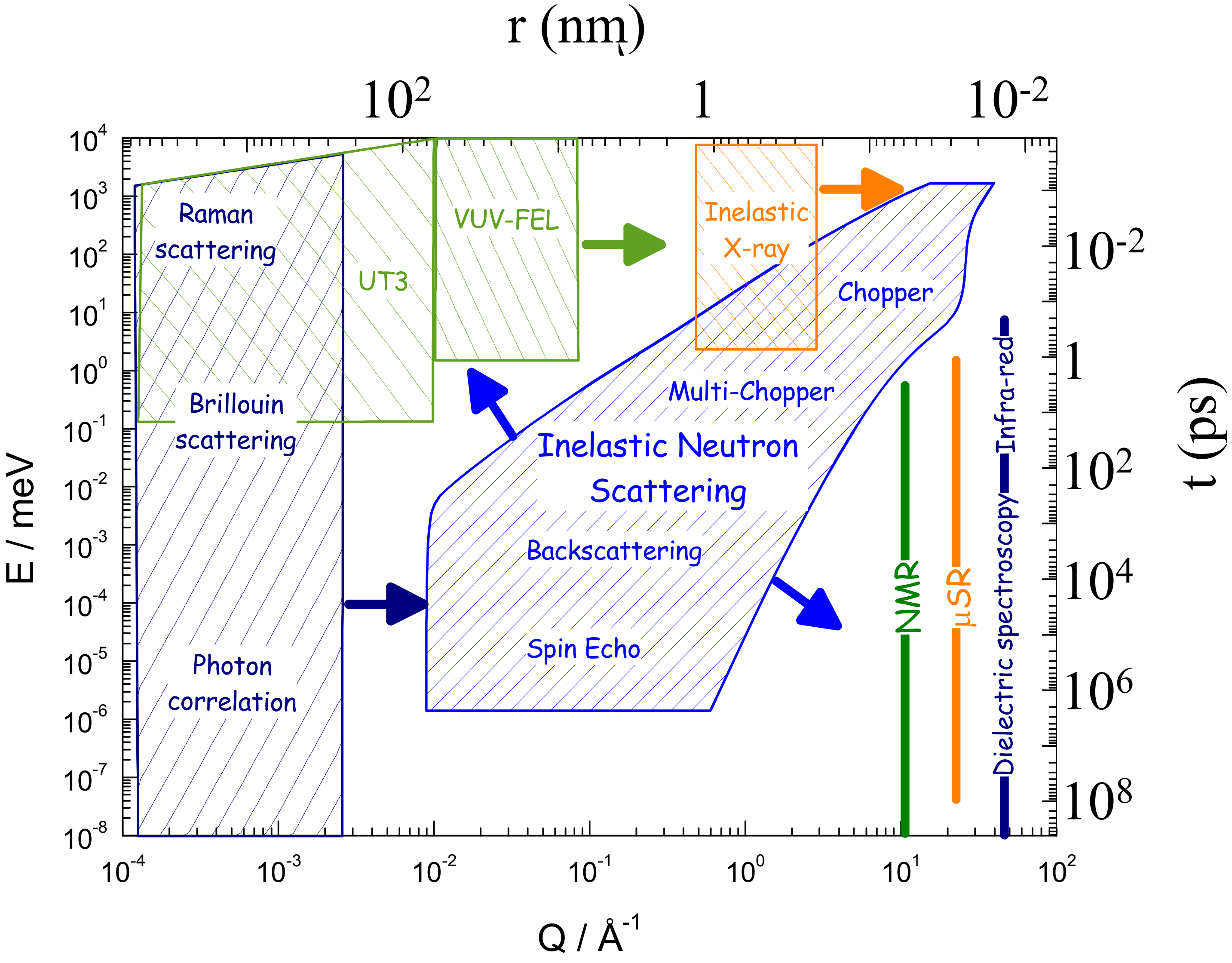
- Neutrons interacting with nuclei
  - Absorption by nuclei
    - Cross section (i.e. absorption probability) for thermal neutrons usually ~1/v, with resonances at high energy (> keV)
  - Scattering by nuclei
    - Coherent scattering – scattering from different nuclei add in phase
    - Incoherent scattering – random phases between scattering from different nuclei

- Neutrons interacting with magnetic fields
  - Magnetic dipolar interaction
    - Scattering from magnetic field (B) due to unpaired electrons – coherent

Neutron Scattering Complements Other Techniques in Length Scale….



……and Time Scale



The Neutron has Both Particle-Like and Wave-Like Properties

- Mass: $m_n = 1.675 \times 10^{-27}$ kg
- Charge = 0; Spin = ½
- Magnetic dipole moment: $\mu_n = - 1.913\ \mu_N$
- Nuclear magneton: $\mu_N = eh/4\pi m_p = 5.051 \times 10^{-27}$ J T^{-1}
- Velocity (v), kinetic energy (E), wavevector (k), wavelength (λ), temperature (T).
- $E = m_n v^2/2 = k_B T = (hk/2\pi)^2/2m_n$; $k = 2\pi/\lambda = m_n v/(h/2\pi)$

	Energy (meV)	**Temp (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**

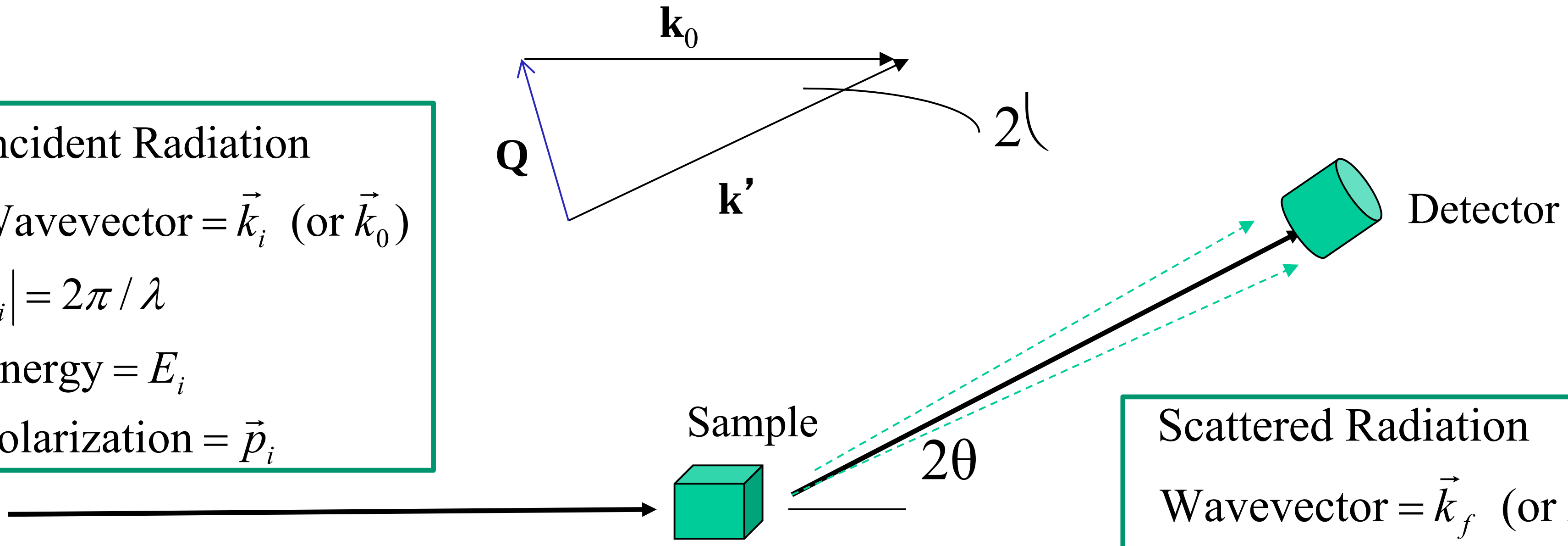
λ (nm) = 395.6 / v (m/s)

E (meV) = 0.02072 k^2 (k in nm^{-1})

Advantages & Disadvantages of Neutrons

- Advantages ☺
  - λ similar to interatomic spacings
  - Penetrates bulk matter
  - Strong contrast possible
  - Energy similar to that of elementary excitations (phonons, magnons etc)
  - Scattering strongly by magnetic fields
  - Data interpretation is direct
- Disadvantages ☹
  - Low brilliance of neutron sources
  - Some elements absorb neutrons strongly
  - Kinematic restrictions on Q for large energy transfers
  - Difficult to study excitations at high (eV) energies
  - Provides statistical averages rather than real space pictures

A Typical Scattering Experiment



Incident Radiation

Wavevector $= \vec{k}_i$ (or $\vec{k}_0$)

$|k_i| = 2\pi / \lambda$

Energy $= E_i$

Polarization $= \vec{p}_i$

Scattered Radiation

Wavevector $= \vec{k}_f$ (or $\vec{k}'$)

Energy $= E_f$

Polarization $= \vec{p}_f$

Wavevector Transfer, $\vec{Q} = \vec{k}_f - \vec{k}_i$

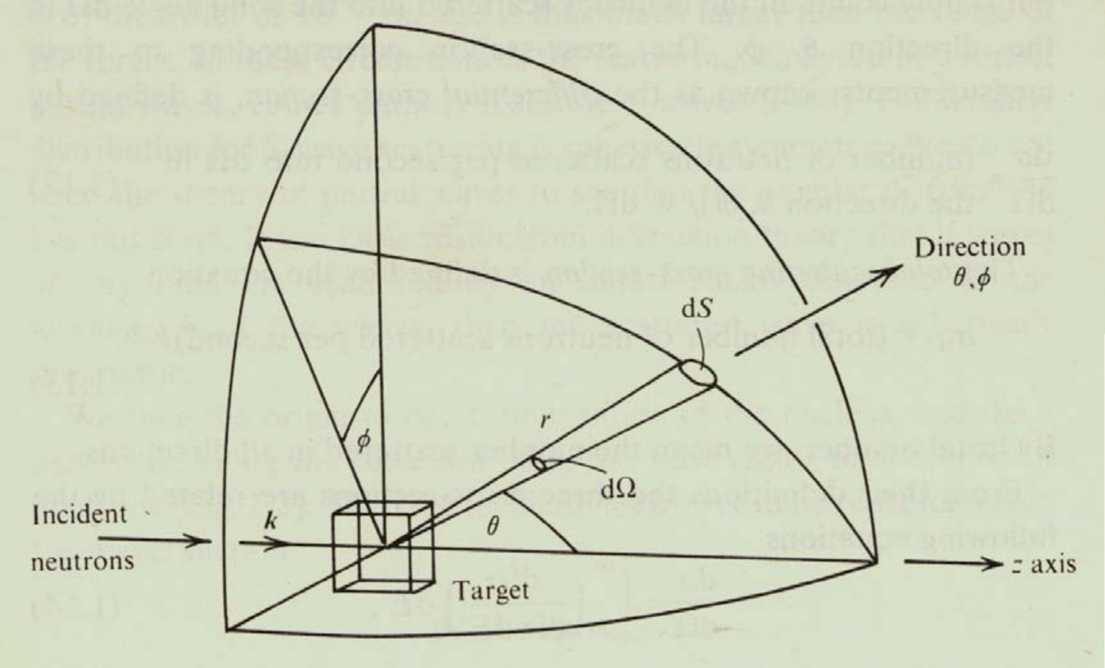
Energy Transfer, $\Delta E = h\upsilon = \hbar\omega = E_f - E_i$

For x-rays: $\Delta E << E_f$ or E_i so $Q = 2k_i \sin\theta$

Polarization, $\vec{p}_i \rightarrow \vec{p}_f$

Notice that the finite size of the detector and sample imply uncertainty in the direction of the wavevectors

Cross Sections



cross section

The effective area presented by a nucleus to an incident neutron. One unit for cross section is the barn, as in "can't hit the side of a barn!"

$$\Phi = \text{number of incident neutrons per cm}^2 \text{ per second}$$

$$\sigma = \text{total number of neutrons scattered per second} / \Phi$$

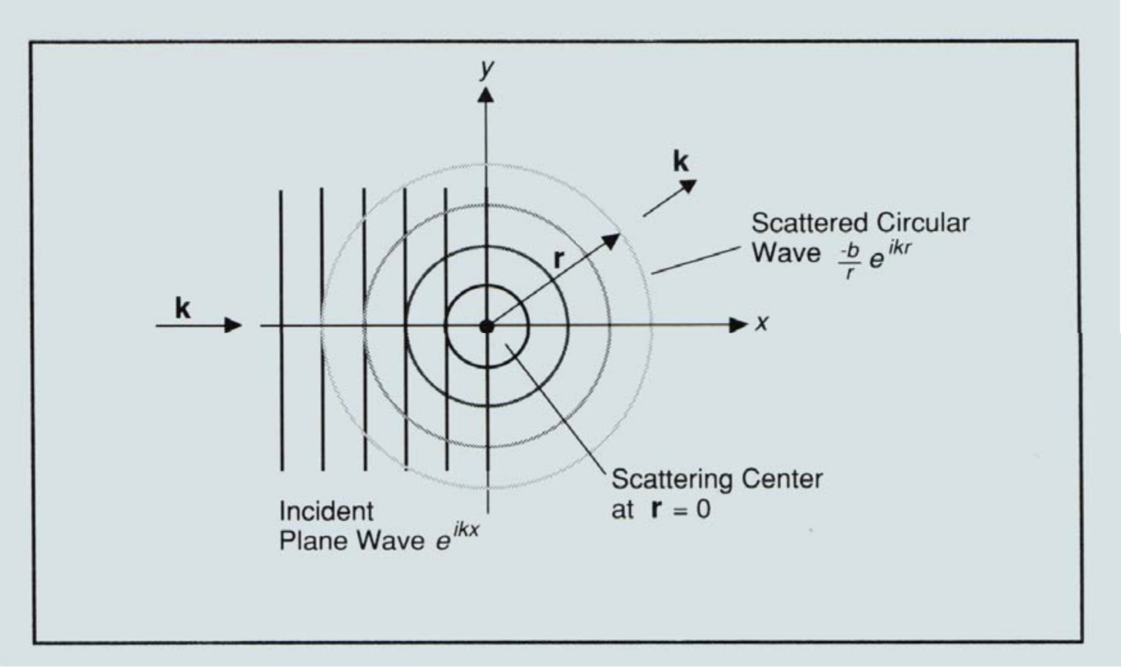
$$\frac{d\sigma}{d\Omega} = \frac{\text{number of neutrons scattered per second into } d\Omega}{\Phi \, d\Omega}$$

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

∫ measured in barns:
1 barn = 10^{-24} cm^2

Attenuation = exp(-N ∫t)
N = # of atoms/unit volume
t = thickness

Neutron Scattering by a Single (fixed) Nucleus



- range of nuclear force (~ 1fm) is << neutron wavelength so scattering is "point-like"
- energy of neutron is too small to change energy of nucleus & neutron cannot transfer KE to a fixed nucleus => scattering is elastic
- we consider only scattering far from nuclear resonances where neutron absorption is negligible

If v is the velocity of the neutron (same before and after scattering), the number of neutrons passing through an area dS per second after scattering is :

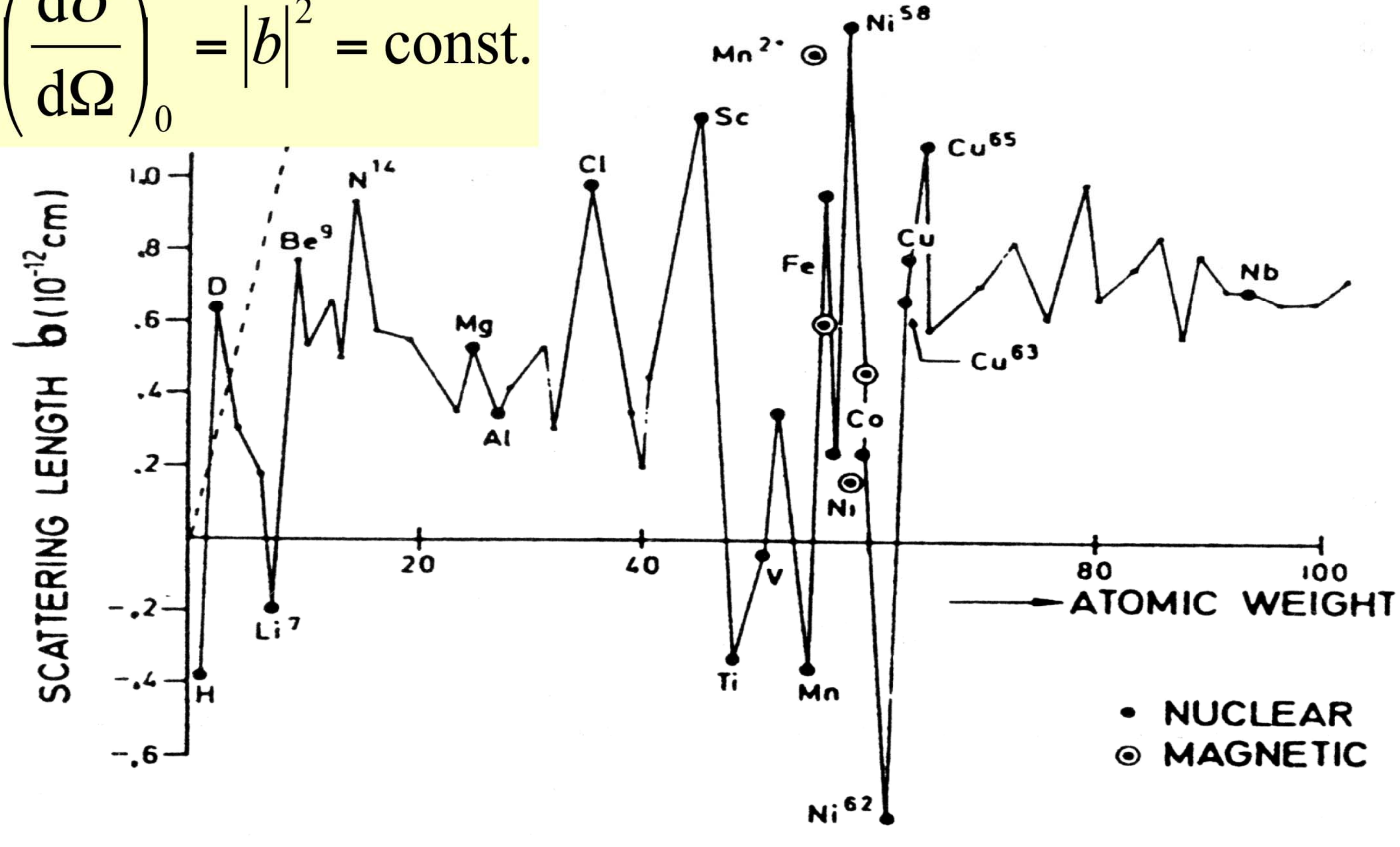
$$\mathrm{v\ dS}\left|\psi_{\mathrm{scat}}\right|^2 = \mathrm{v\ dS\ b^2/r^2 = v\ b^2\ d\Omega}$$

Since the number of incident neutrons passing through unit areas is : $\Phi = \mathrm{v}\left|\psi_{\mathrm{incident}}\right|^2 = \mathrm{v}$

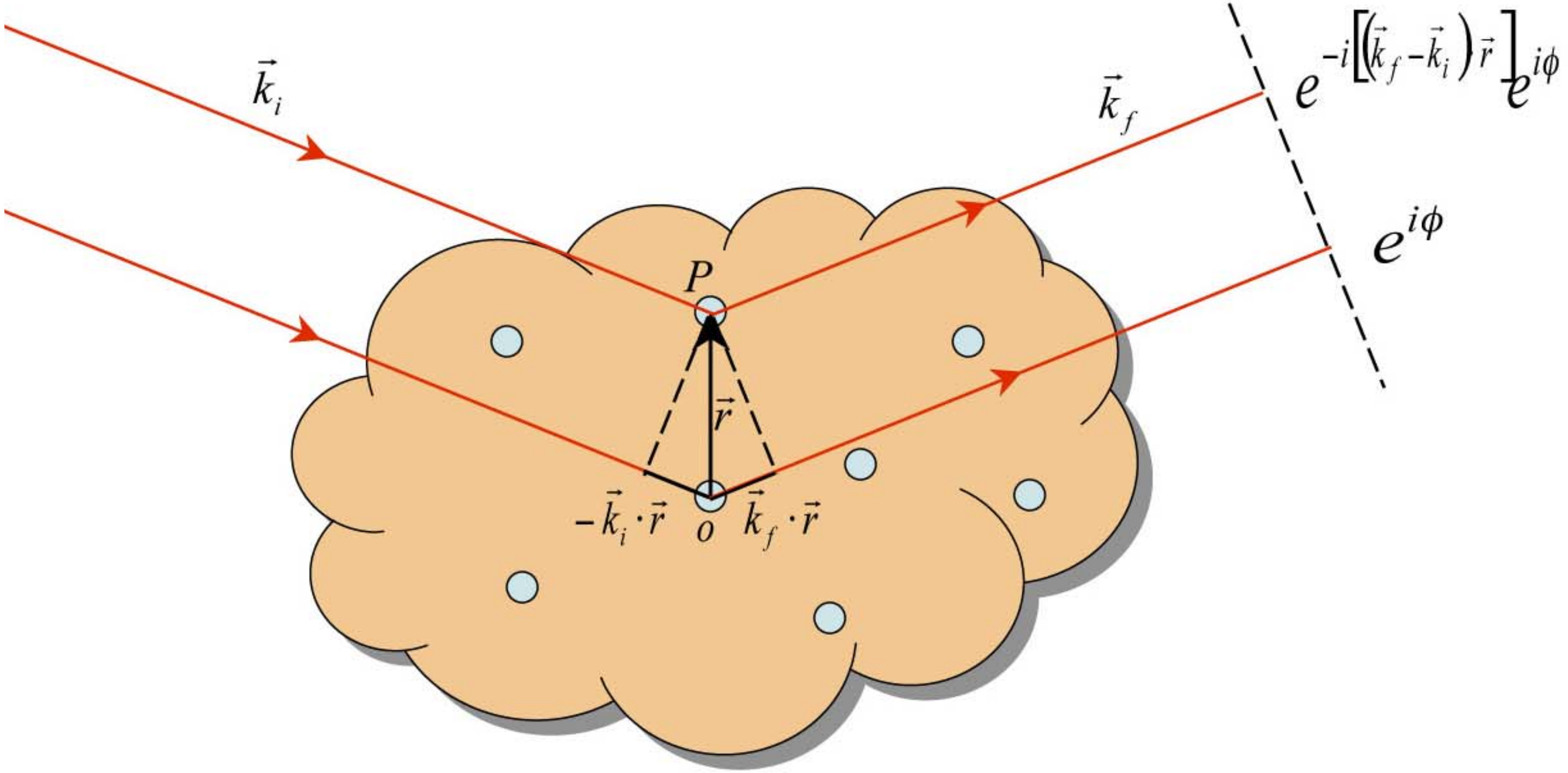
$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \frac{\mathrm{v\ b^2\ d\Omega}}{\Phi \mathrm{d}\Omega} = \mathrm{b}^2 \qquad \text{so } \sigma_{\mathrm{total}} = 4\pi b^2 \qquad \text{(note units)}$$

Intrinsic Cross Section: Neutrons

$$\left(\frac{d\sigma}{d\Omega}\right)_0 = |b|^2 = \text{const.}$$



Adding up phases at the detector of the wavelets scattered from all the scattering centers in the sample:



Adding up Neutrons Scattered by Many Nuclei

At a scattering center located at $\vec{R}_i$ the incident wave is $e^{\,i\,\vec{k}_0.\vec{R}_i}$

so the scattered wave at $\vec{r}$ is $\psi_{\text{scat}} = \sum e^{i\,\vec{k}_0.\vec{R}_i}\left[\frac{-b_i}{|\vec{r}-\vec{R}_i|}e^{i\vec{k}'.(\vec{r}-\vec{R}_i)}\right]$

$$\therefore \frac{d\sigma}{d\Omega} = \frac{vdS|\psi_{scat}|^2}{vd\Omega} = \frac{dS}{d\Omega}\left|b_i e^{i\vec{k}'.\vec{r}}\sum\frac{1}{|\vec{r}-\vec{R}_i|}e^{i\,(\vec{k}_0-\vec{k}').\vec{R}_i}\right|^2$$

(using defn. from earlier VG)

If we measure far enough away so that $r >> R_i$ we can use $d\Omega = dS/r^2$ to get

$$\boxed{\frac{d\sigma}{d\Omega} = \sum_{i,j} b_i b_j e^{i(\vec{k}_0-\vec{k}').(\vec{R}_i-\vec{R}_j)} = \sum_{i,j} b_i b_j e^{-i\vec{Q}.(\vec{R}_i-\vec{R}_j)}}$$

where the wavevector transfer Q is defined by $\vec{Q} = \vec{k}' - \vec{k}$

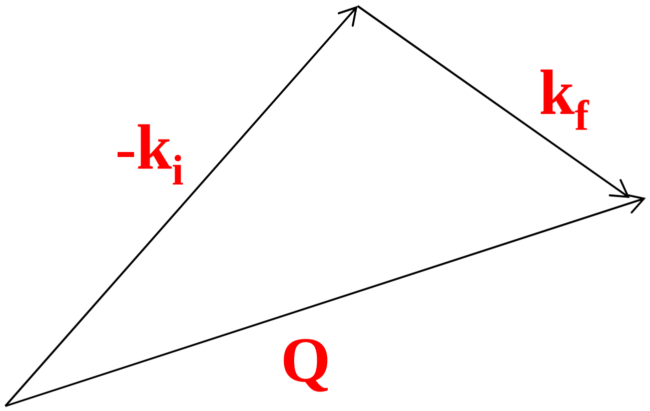
Note: we have assumed the scattering centers don’t move

The Scattering Triangle

- The wavevector transfer, variously denoted Q or q, is defined by:

$$\vec{Q} = \vec{k}_i - \vec{k}_f$$

- The scattering triangle defines the vector relationship between these quantities



Coherent and Incoherent Scattering of Neutrons

The scattering length, b_i , depends on the nuclear isotope, spin relative to the neutron & nuclear eigenstate. For a single nucleus:

$$b_i = \langle b \rangle + \delta b_i \quad \text{where } \delta \mathrm{b}_\mathrm{i} \text{ averages to zero}$$

$$b_i b_j = \langle b \rangle^2 + \langle b \rangle (\delta b_i + \delta b_j) + \delta b_i \delta b_j$$

$$\text{but } \langle \delta b \rangle = 0 \ \text{ and } \langle \delta b_i \delta b_j \rangle \text{ vanishes unless i = j}$$

$$\langle \delta b_i^2 \rangle = \langle b_i - \langle b \rangle \rangle^2 = \langle b^2 \rangle - \langle b \rangle^2$$

$$\therefore \frac{d\sigma}{d\Omega} = \langle b \rangle^2 \sum_{i,j} e^{-i\vec{Q}.(\vec{R}_i - \vec{R}_j)} + (\langle b^2 \rangle - \langle b \rangle^2) N$$

Coherent Scattering
(scattering depends on the direction & magnitude of **Q**)

Incoherent Scattering
(scattering is uniform in all directions)

Note: N = number of atoms in scattering system

Nuclear Spin Incoherent Scattering

Consider a single isotope with spin I. The spin of the nucleus - neutron system can be $(I+1/2)$ or $(I-1/2)$.

The number of states with spin $(I+1/2)$ is $2(I+1/2)+1=2I+2$

The number of states with spin $(I-1/2)$ is $2(I-1/2)+1=2I$

If the neutrons and the nuclear spins are unpolarized, each spin state has the same *a priori* probability.

The frequency of occurence of b^+ state is $f^+=(2\mathrm{I}+2)/(4\mathrm{I}+2)$

The frequency of occurence of b^- state is $f^-=(2\mathrm{I})/(4\mathrm{I}+2)$

Thus $\langle b\rangle=\dfrac{1}{2I+1}\left[(I+1)b^++Ib^-\right]$ and $\langle \mathrm{b}^2\rangle=\dfrac{1}{2I+1}\left[(I+1)(b^+)^2+I(b^-)^2\right]$

Values of $\int_{coh}$ and $\int_{inc}$

Nuclide	$\int_{coh}$	$\int_{inc}$	Nuclide	$\int_{coh}$	$\int_{inc}$
^{1}H	1.8	80.2	V	0.02	5.0
^{2}H	5.6	2.0	Fe	11.5	0.4
C	5.6	0.0	Co	1.0	5.2
O	4.2	0.0	Cu	7.5	0.5
Al	1.5	0.0	^{36}Ar	24.9	0.0

- Difference between H and D used in experiments with soft matter (contrast variation)
- Al used for windows
- V used for sample containers in diffraction experiments and as calibration for energy resolution
- Fe and Co have nuclear cross sections similar to the values of their magnetic cross sections
- Find scattering cross sections at the NIST web site at:
  http://webster.ncnr.nist.gov/resources/n-lengths/

Coherent Elastic Scattering measures the Structure Factor S(Q) i.e. correlations of atomic positions

$\frac{d\sigma}{d\Omega} = \langle b \rangle^2 N.S(\vec{Q})$ for an assembly of similar atoms where $S(\vec{Q}) = \frac{1}{N}\left\langle \sum_{i,j} e^{-i\vec{Q}.(\vec{R}_i - \vec{R}_j)} \right\rangle_{\text{ensemble}}$

Now $\sum_i e^{-i\vec{Q}.\vec{R}_i} = \int d\vec{r}.e^{-i\vec{Q}.\vec{r}} \sum_i \delta(\vec{r} - \vec{R}_i) = \int d\vec{r}.e^{-i\vec{Q}.\vec{r}} \rho_N(\vec{r})$ where ρ_N is the nuclear number density

so
$$\boxed{S(\vec{Q}) = \frac{1}{N}\left\langle \left| \int d\vec{r}.e^{-i\vec{Q}.\vec{r}} \rho_N(\vec{r}) \right|^2 \right\rangle}$$

or $S(\vec{Q}) = \frac{1}{N}\int d\vec{r}\,'\int d\vec{r}.e^{-i\vec{Q}.(\vec{r}-\vec{r}\,')} \left\langle \rho_N(\vec{r})\rho_N(\vec{r}\,') \right\rangle = \frac{1}{N}\int d\vec{R}\int d\vec{r} e^{-i\vec{Q}.\vec{R}} \left\langle \rho_N(\vec{r})\rho_N(\vec{r}-\vec{R}) \right\rangle$

ie
$$\boxed{S(\vec{Q}) = 1 + \int d\vec{R}.\{g(\vec{R}) - \bar{\rho}\}.e^{-i\vec{Q}.\vec{R}}}$$

where $\boxed{g(\vec{R}) = \sum_{i \neq 0} \left\langle \delta(\vec{R} - \vec{R}_i + \vec{R}_0) \right\rangle}$ is a function of $\vec{R}$ only.

g(R) is known as the **static pair correlation function**. It gives the probability that there is an atom, i, at distance R from the origin of a coordinate system, given that there is also a (different) atom at the origin of the coordinate system at the same instant in time.

S(Q) and g(r) for Simple Liquids

- Note that S(Q) and g(r)/〉 both tend to unity at large values of their arguments
- The peaks in g(r) represent atoms in "coordination shells"
- g(r) is expected to be zero for r < particle diameter – ripples are truncation errors from Fourier transform of S(Q)

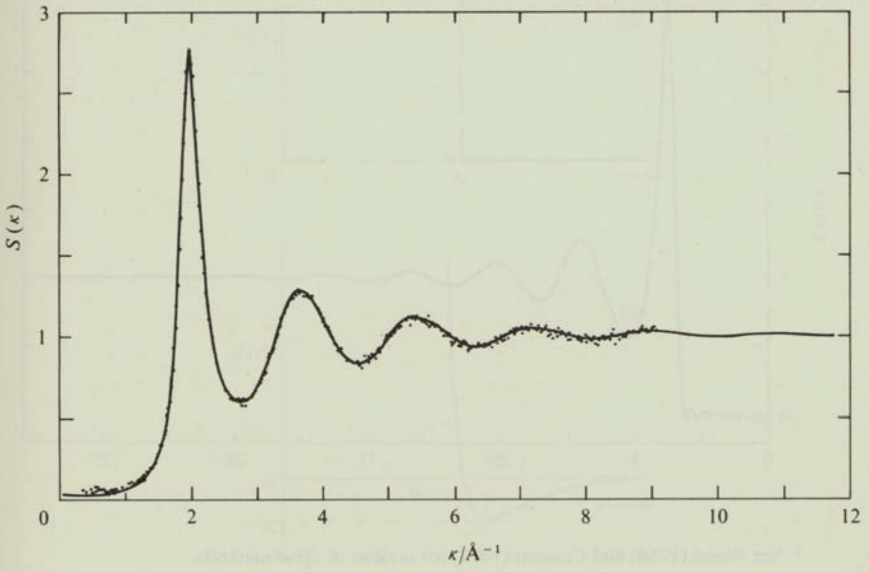


Fig. 5.1 The structure factor $S(\kappa)$ for ^{36}Ar at 85 K. The curve through the experimental points is obtained from a molecular dynamics calculation of Verlet based on a Lennard-Jones potential. (After Yarnell *et al.*, 1973.)

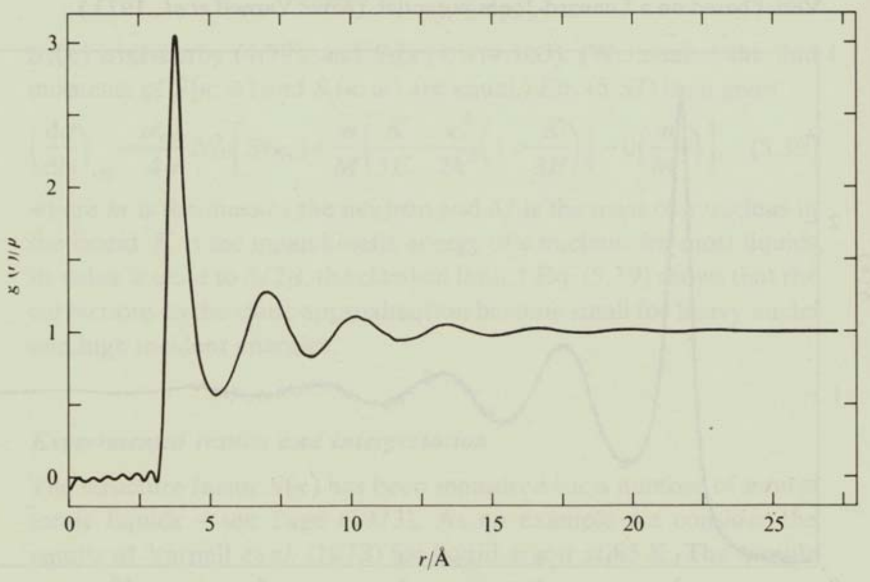
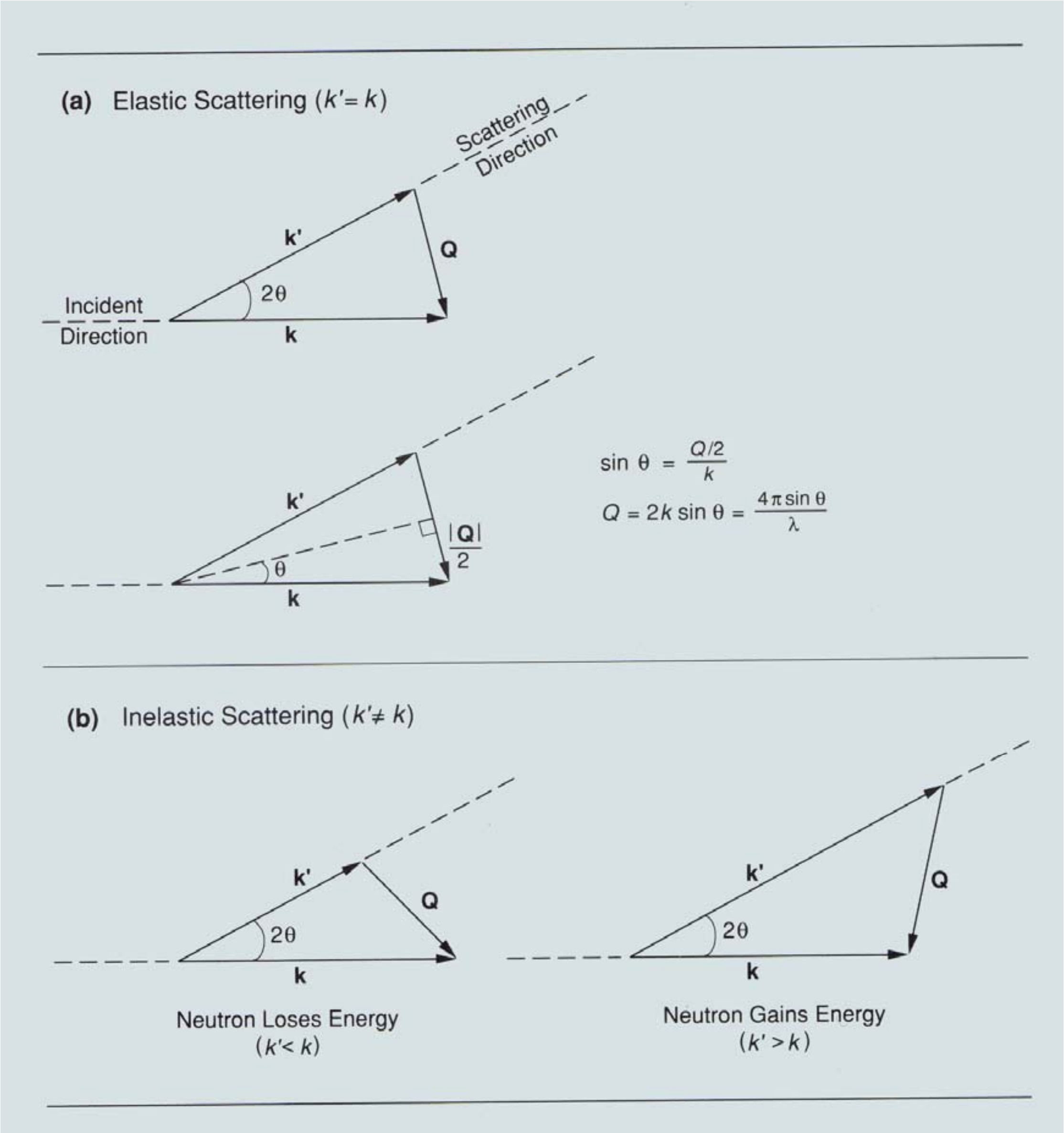
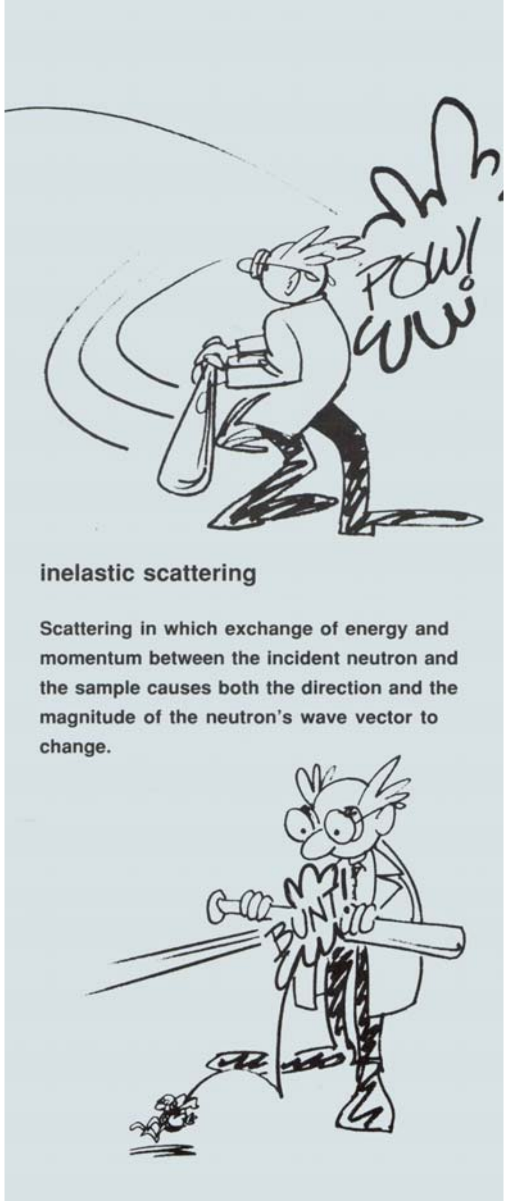


Fig. 5.2 The pair-distribution function $g(r)$ obtained from the experimental results in Fig. 5.1. The mean number density is $\rho = 2.13 \times 10^{28}$ atoms m^{-3}. (After Yarnell *et al.*, 1973.)

Neutrons can also gain or lose energy in the scattering process: this is called inelastic scattering





inelastic scattering

Scattering in which exchange of energy and momentum between the incident neutron and the sample causes both the direction and the magnitude of the neutron's wave vector to change.

The Elastic & Inelastic Scattering Cross Sections Have an Intuitive Similarity

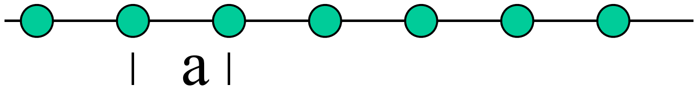
- The intensity of elastic, coherent neutron scattering is proportional to the spatial Fourier Transform of the Pair Correlation Function, G(r) I.e. the probability of finding a particle at position r if there is simultaneously a particle at r=0

- The intensity of inelastic coherent neutron scattering is proportional to the space *and time* Fourier Transforms of the *time-dependent* pair correlation function function, G(r,t) = probability of finding a particle at position r *at time t* when there is a particle at r=0 and *t=0*.

- For inelastic *incoherent* scattering, the intensity is proportional to the space and time Fourier Transforms of the *self-correlation* function, $G_s(r,t)$ I.e. the probability of finding a particle at position r at time t when *the same* particle was at r=0 at t=0

Diffraction from a Frozen Wave

- Recall that $S(\vec{Q}) = \frac{1}{N}\left|\sum_k e^{i\vec{Q}.\vec{r}_k}\right|^2$

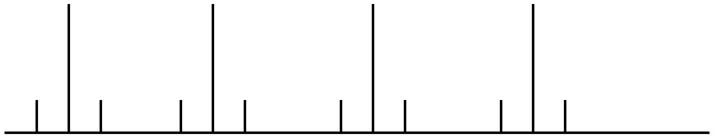


- We know that for a linear chain of “atoms” along the x axis, $S(Q_x)$ is just a series of delta function reciprocal lattice planes at $Q_x = n2\pi/a$, where a is the separation of atoms

What happens if we put a "frozen" wave in the chain of atoms so that the atomic positions are $x_p = pa + u\cos kpa$ where p is an integer and u is small?

$$S(Q) = \left|\sum_p e^{iQpa} e^{iQu\cos kpa}\right|^2 \approx \left|\sum_p e^{iQpa}(1 + iQu[e^{ikpa} + e^{-ikpa}])\right|^2$$

$$\approx \left|\sum_p e^{iQpa} + iQu[e^{i(Q+k)pa} + e^{i(Q-k)pa}]\right|^2$$



so that in addition to the Bragg peaks we get weak satellites at $Q = G \pm k$

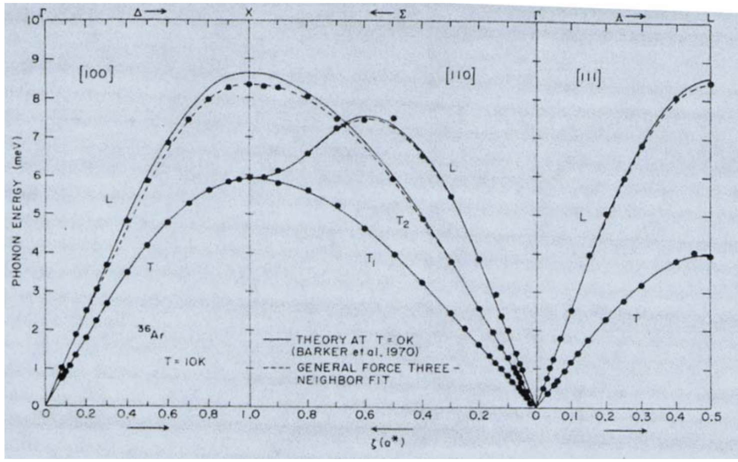
What Happens if the Wave Moves?

- If the wave moves through the chain, the scattering still occurs at wavevectors G + k and G – k but now the scattering is inelastic

- For quantized lattice vibrations, called phonons, the energy change of the neutron is $\hbar\omega$ where ω is the vibration frequency.

- In a crystal, the vibration frequency at a given value of $\vec{q}$ (called the phonon wavevector) is determined by interatomic forces. These frequencies map out the so-called phonon dispersion curves.

- Different branches of the dispersion curves correspond to different types of motion



phonon dispersion in ^{36}Ar

A Phonon is a Quantized Lattice Vibration

- Consider linear chain of particles of mass M coupled by springs. Force on n’th particle is

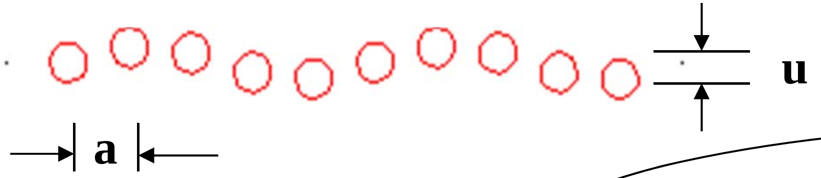
$$F_n = \alpha_0 u_n + \alpha_1 (u_{n-1} + u_{n+1}) + \alpha_2 (u_{n-2} + u_{n+2}) + \ldots$$

First neighbor force constant

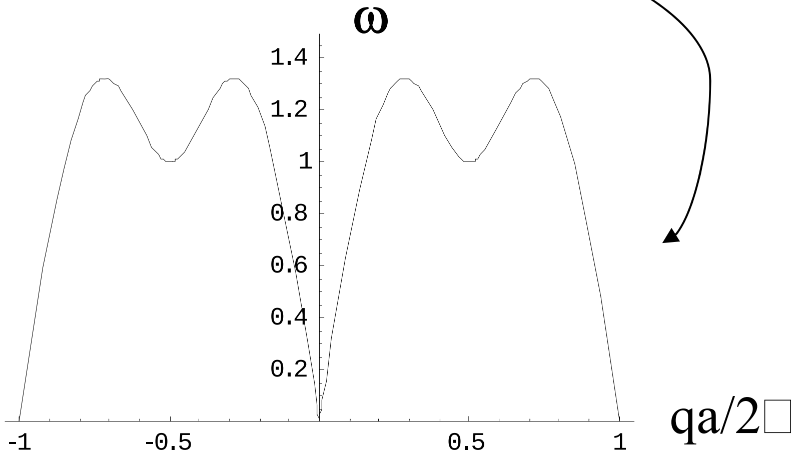
displacements

- Equation of motion is $F_n = M\ddot{u}_n$
- Solution is: $u_n(t) = A_q e^{i(qna - \omega t)}$ with $\omega_q^2 = \frac{4}{M} \sum_{\nu} \alpha_\nu \sin^2(\frac{1}{2}\nu q a)$

$$q = 0, \pm\frac{2\pi}{L}, \pm\frac{4\pi}{L}, \ldots\ldots \pm\frac{N}{2}\frac{2\pi}{L}$$

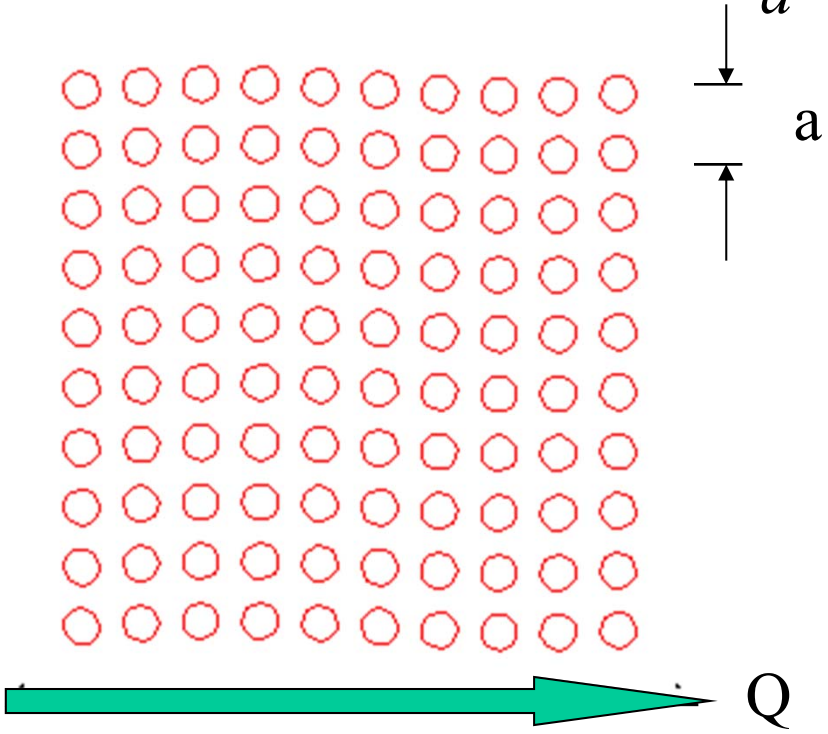


Phonon Dispersion Relation:
Measurable by inelastic neutron scattering



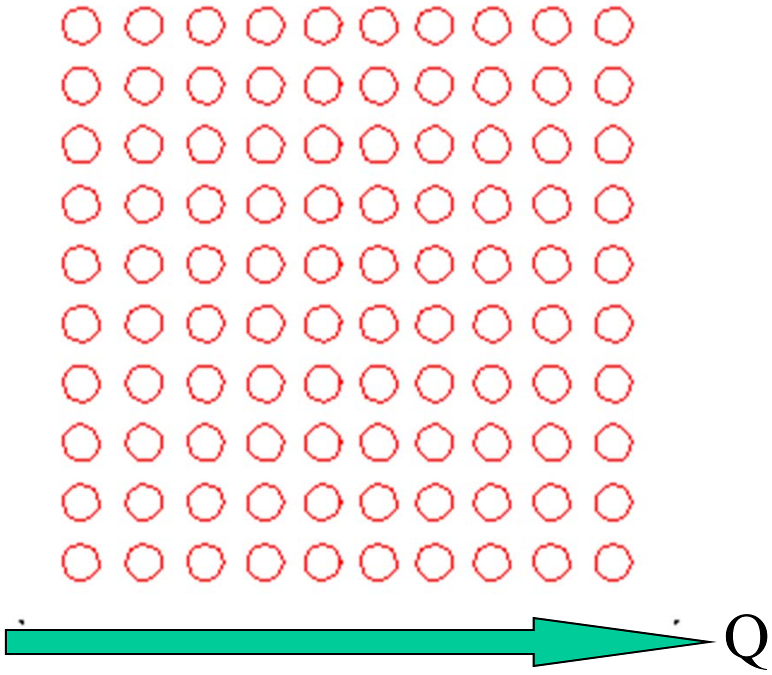
Atomic Motions for Longitudinal & Transverse Phonons

$$\vec{Q}=\frac{2\pi}{a}(0.1,0,0)$$



Transverse phonon

$$\vec{e}_T=(0,0.1,0)a$$

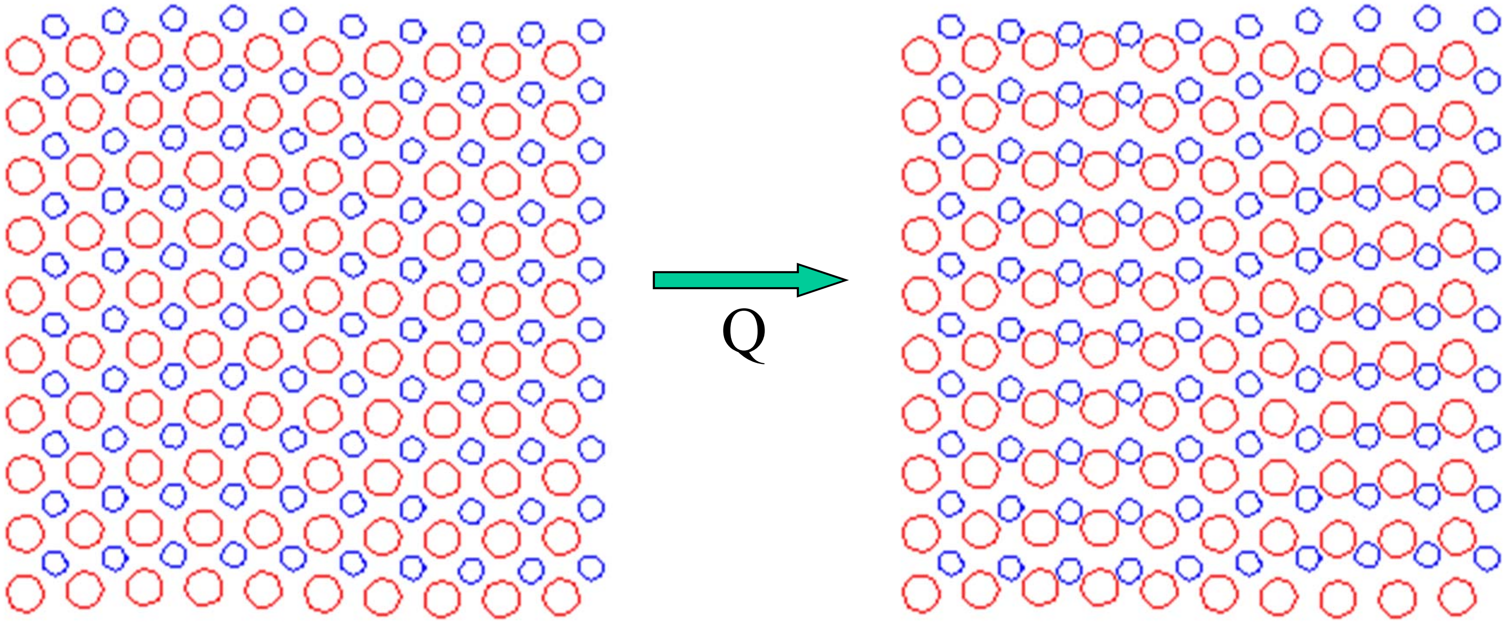


Longitudinal phonon

$$\vec{e}_L=(0.1,0,0)a$$

$$\vec{R}_l=\vec{R}_{l0}+\vec{e}_s e^{i(\vec{Q}.\vec{R}_l-\omega t)}$$

Transverse Optic and Acoustic Phonons



Acoustic

$$\vec{e}_{red} = (0,0.1,0)a$$

$$\vec{e}_{blue} = (0,0.14,0)a$$

Optic

$$\vec{e}_{red} = (0,0.1,0)a$$

$$\vec{e}_{blue} = (0,-0.14,0)a$$

$$\vec{R}_{lk} = \vec{R}_{lk}^{0} + \vec{e}_s e^{i(\vec{Q}.\vec{R}_l - \omega t)}$$

General Expression for $d^2\sigma/d\Omega dE$

- Squires (eqn 2.59) derives the following expression:

$$\boxed{\frac{d^2\sigma}{d\Omega dE'} = \frac{k'}{k}\frac{1}{2\pi\hbar}\sum_{i,i'} b_i b'_{i'} \int_{-\infty}^{\infty} \left\langle e^{-i\vec{Q}.\vec{R}_{i'}(0)} e^{i\vec{Q}.\vec{R}_i(t)} \right\rangle e^{-i\omega t}\, dt}$$

where $\vec{R}_i(t)$ is a Heisenberg operator i.e.

$e^{-i\vec{Q}.\vec{R}_i(t)} = e^{iHt/\hbar} e^{-i\vec{Q}.\vec{R}_i} e^{-iHt/\hbar}$ where H is the Hamiltonian of the scatterer

and $\langle\ \rangle$ denotes a thermal average over the possible states, λ, of the

scatterer -- i.e. for any operator, $\langle \mathrm{A} \rangle = \sum_{\lambda} p_\lambda \langle \lambda | A | \lambda \rangle$

- Note that, because of the operators and the average over the states of the system, this expression is not easy to evaluate in the general case

- Note also that the exponential operators do not commute – each contains H and therefore p, and p and R do not commute.

Correlation Functions

$$\text{Suppose we define:}\quad G(\vec{r},t) = \frac{1}{(2\pi)^3}\frac{1}{N}\int e^{-i\vec{Q}'.\vec{r}}\sum_{j,j'}\left\langle e^{-i\vec{Q}'.\vec{R}_{j'}(0)}e^{i\vec{Q}'.\vec{R}_j(t)}\right\rangle d\vec{Q}'$$

$$\text{and}\quad S(\vec{Q},\omega) = \frac{1}{2\pi\hbar}\int G(\vec{r},t)e^{i(\vec{Q}.\vec{r}-\omega t)}d\vec{r}.dt \qquad \text{then we find}$$

$$\left(\frac{d^2\sigma}{d\Omega dE'}\right)_{coh} = b_{coh}^2\frac{k'}{k}NS(\vec{Q},\omega)\ \text{ provided there is only one type of atom}$$

Squires (eqn 4.14 to 4.17) shows that

$$\boxed{G(\vec{r},t) = \frac{1}{N}\sum_{j,j'}\int\left\langle \delta\{\vec{r}'-\vec{R}_{j'}(0)\}\delta\{\vec{r}'+\vec{r}-\vec{R}_j(t)\}\right\rangle d\vec{r}'}$$

- Note again that the operators do not commute. If we ignore this fact, we can do the integration and obtain

$$\boxed{G_{classical}(\vec{r},t) = \frac{1}{N}\sum_{j,j'}\left\langle \delta\{\vec{r}-\vec{R}_j(t)+\vec{R}_{j'}(0)\}\right\rangle}$$

Correlation Functions (cont’d)

$$G_{classical}(\vec{r},t)=\frac{1}{N}\sum_{j,j'}\left\langle \delta\{\vec{r}-\vec{R}_{j}(t)+\vec{R}_{j'}(0)\}\right\rangle$$

- We expressed the coherent scattering cross section in terms of G(**r**,t)

- If we use the classical variant given above, there is a clear physical meaning – G(**r**,t) is the probability that if particle j’ is at the origin at time zero, particle j will be at position **r** at time t.

- We can do the same thing with the incoherent scattering and express it in terms of a self-correlation function whose classical version is

$$G_{classical}^{self}(\vec{r},t)=\left\langle \delta\{\vec{r}-R_{j}(t)+R_{j}(0)\}\right\rangle$$

- This says that the incoherent scattering is related to the probability that if a particle is at the origin at time zero, *the same* particle will be at position **r** at time t.

Inelastic Neutron Scattering Measures Atomic Motions

In term of the pair correlation functions, one finds

$$\left(\frac{d^2\sigma}{d\Omega.dE}\right)_{coh} = b_{coh}^2\frac{k'}{k}NS(\vec{Q},\omega)$$

$$\left(\frac{d^2\sigma}{d\Omega.dE}\right)_{inc} = b_{inc}^2\frac{k'}{k}NS_s(\vec{Q},\omega)$$

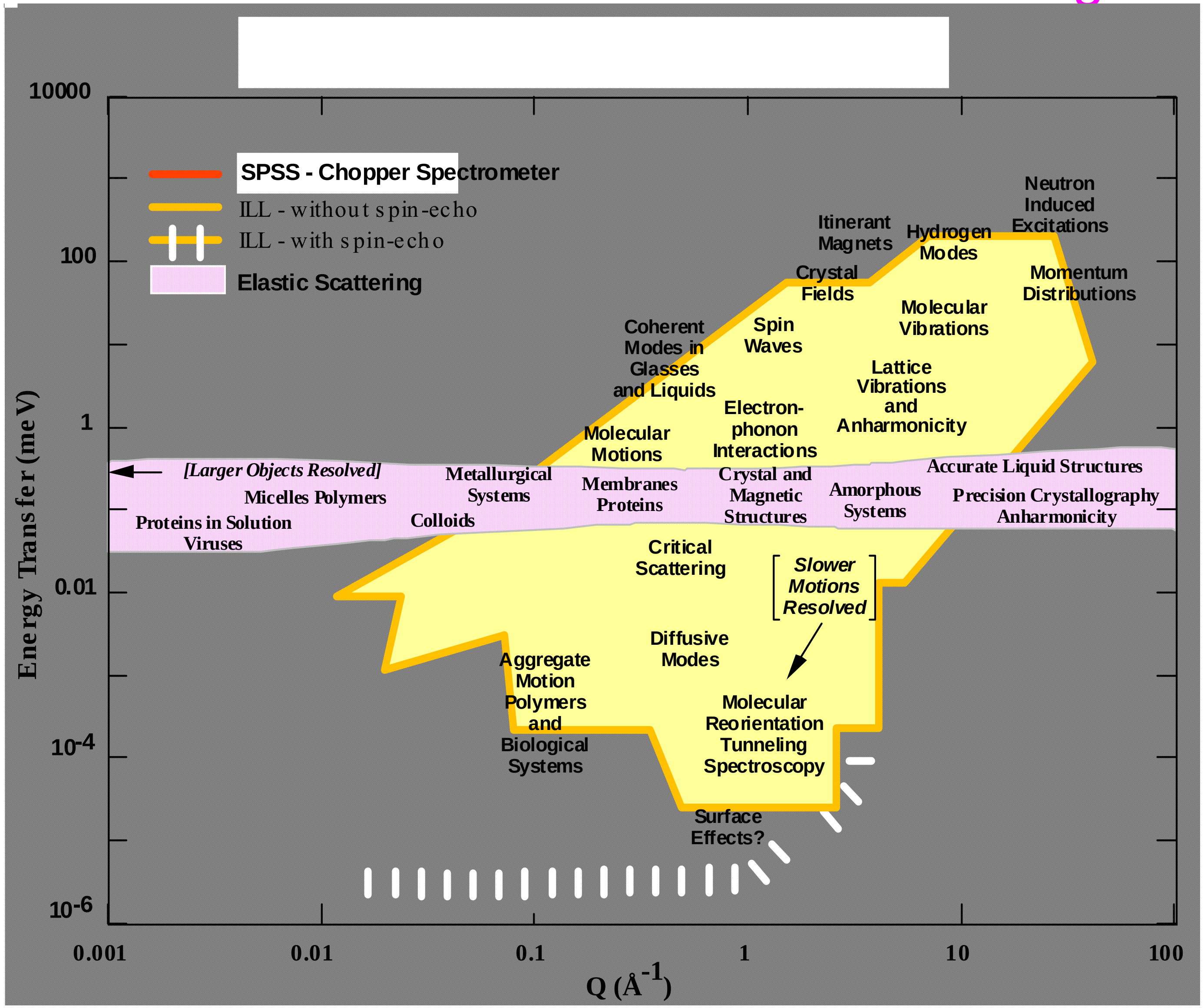
(h/2□)**Q** & (h/2□)⌉ are the momentum & energy transferred to the neutron during the scattering process

where

$$S(\vec{Q},\omega) = \frac{1}{2\pi\hbar}\iint G(\vec{r},t)e^{i(\vec{Q}.\vec{r}-\omega t)}d\vec{r}dt \quad \text{and} \quad S_s(\vec{Q},\omega) = \frac{1}{2\pi\hbar}\iint G_s(\vec{r},t)e^{i(\vec{Q}.\vec{r}-\omega t)}d\vec{r}dt$$

- Inelastic coherent scattering measures *correlated* motions of different atoms
- Inelastic incoherent scattering measures *self-correlations* e.g. diffusion

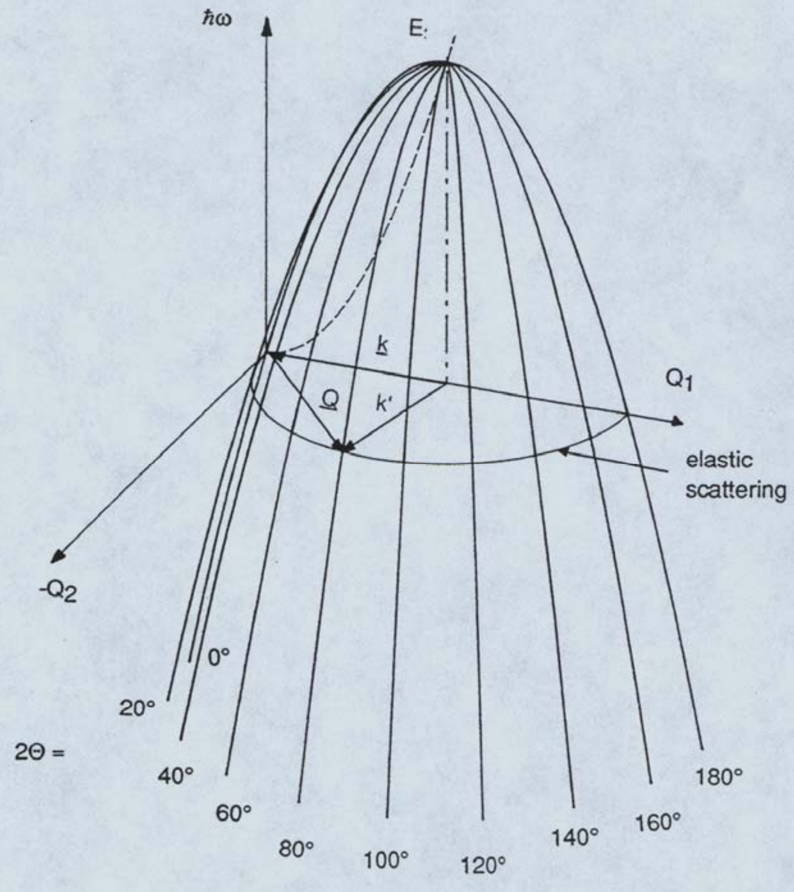
Much of the Scientific Impact of Neutron Scattering Has Involved the Measurement of Inelastic Scattering

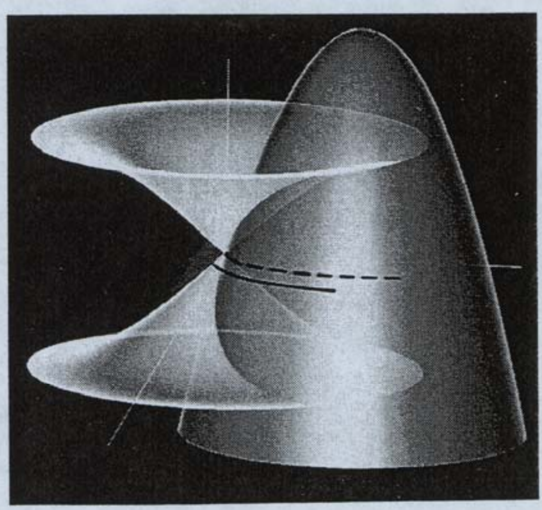


Energy & Wavevector Transfers accessible to Neutron Scattering

The Accessible Energy and Wavevector Transfers Are Limited by Conservation Laws

- Neutron cannot lose more than its initial kinetic energy & momentum must be conserved





Intersection of the dynamical range surface (paraboloid) with a (rotationally symmetric) dispersion surface. The projection of the lines of intersection into the Q-plane are different for energy gain and energy loss

The Kinematic Approximation

- Note that the approximation we have just seen ignores
  - Depletion of the incident beam by scattering or absorption
  - Multiple scattering

  i.e. energy is not conserved

- This so-called “kinematic approximation” is OK for weak scattering, very small crystals or “bad” crystals

- It is usually used for interpreting diffraction experiments, though “extinction corrections” are often needed with single crystals
  - If it’s not adequate, use dynamical theory

Magnetic Properties of the Neutron

- The neutron has a magnetic moment of -9.649 x 10^{-27} JT^{-1}

  $$\vec{\mu}_n = -\gamma \mu_N \vec{\sigma}$$

  where $\mu_N = {e\hbar}/{2m_p}$ is the nuclear magneton,

  $m_p =$ proton mass, $e =$ proton charge and $\gamma = 1.913$

  $\vec{\sigma}$ is the Pauli spin operator for the neutron. Its eignevalues are ± 1

- Note that the neutron's spin and magnetic moment are antiparallel
- Because of its magnetic moment, the neutron feels a potential given by:

$$V_m(\vec{r}) = -\vec{\mu}_n . \vec{B}(\vec{r}) \quad \text{where} \quad \vec{B}(\vec{r}) = \mu_0 \mu \vec{H}(\vec{r}) = \mu_0 [\vec{H}(\vec{r}) + \vec{M}(\vec{r})]$$

- Thus the neutron senses the distribution of magnetization in a material
- Homework problems: What is the Zeeman energy in meV of a neutron in a 1 Tesla field? At what temperature is the Boltzmann energy equal to this Zeeman energy? What is the effective scattering length of a "point" magnetic moment of one Bohr magneton?

Magnetic Scattering of the Neutron

- For nuclear scattering, the matrix element that appears in the expression for the scattering cross section is: $\sum_j b_j e^{i\vec{Q}.\vec{R}_j}$

- The equivalent matrix element for magnetic scattering is:

$$\gamma r_0 \frac{1}{2\mu_B} \vec{\sigma}.\vec{M}_\perp(\vec{Q}) \quad \text{where } \mu_B = \frac{e\hbar}{2m_e} \text{ is the Bohr magneton } (9.27 \text{ x } 10^{-24} \text{ JT}^{-1})$$

$$\text{and } r_0 = \frac{\mu_0}{4\pi}\frac{e^2}{m_e} \text{ is classical radius of the electron } (2.818 \text{ x } 10^{-6} \text{ nm})$$

- Here $\vec{M}_\perp(\vec{Q})$ is the component of the Fourier transform of the magnetization that is perpendicular to the scattering vector $\vec{Q}$. This form arises directly from the dipolar nature of the magnetic interaction.

- Unlike the neutron-nucleus interaction, the magnetic interaction of the neutron with a scattering system specifically depends on neutron spin

The Magnetic Scattering Cross Section

- Development of the magnetic scattering cross section follows the same formalism as for the nuclear cross section, with nuclear matrix element replaced by the magnetic interaction matrix element given above

- Need to keep the explicit dependence on neutron spin (or average over neutron spin states for an unpolarized neutron beam).
  - Magnetic scattering may cause a change in the neutron's spin state

- General expressions tend to be complicated, so specific expressions are obtained for various contributions to sample magnetization e.g. unpaired electron spins

- The form of the magnetic cross section implies that neutrons are only sensitive to components of the magnetization that are perpendicular to **Q**.

Scattering by Ions with Unpaired Electrons

- Including only magnetization due to unpaired electron spins and assuming an unpolarized incident neutron beam:

$$\frac{d^2\sigma}{d\Omega.dE} = \frac{(\gamma r_0)^2}{2\pi\hbar}\frac{k'}{k}\sum_{\alpha,\beta}(\delta_{\alpha\beta} - \hat{Q}_\alpha \hat{Q}_\beta)\sum_{ldl'd'} F^*_{d'}(\vec{Q})F_d(\vec{Q})$$

$$\mathrm{x}\int_{-\infty}^{\infty} dt\left\langle \exp\{-i\vec{Q}.\vec{R}_{l'd'}(0)\}\exp\{i\vec{Q}.\vec{R}_{ld}(t)\}\right\rangle.\left\langle S^{\alpha}_{l'd'}(0)S^{\beta}_{ld}(t)\right\rangle e^{-i\omega t}$$

where $F_d(Q)$ is the Fourier transform of the electron spin density around atom *d,* often called the atomic form factor; $S^{〈}$ is the 〈 component of the electron spin and *l,d* labels an atom *d* in unit cell *l*

- This expression can be manipulated to give the scattering cross sections for elastic magnetic scattering inelastic magnetic scattering and magneto-vibrational scattering

What Happens to a Neutron's Spin When the Neutron is Scattered?

- The cross section for magnetic scattering that takes the neutron spin state from σ->σ' and the scattering system from λ->λ' is:

$$\left(\frac{d^2\sigma}{d\Omega.dE}\right)_{\sigma\lambda\to\sigma'\lambda'}=\left(\frac{\gamma r_0}{2\mu_B}\right)^2\frac{k'}{k}\left|\langle\sigma'\lambda'|\vec{\sigma}.\vec{M}_\perp|\sigma\lambda\rangle\right|^2\delta(E_\lambda-E\lambda'+\hbar\omega)$$

- One can show (see Squires) that if $|u\rangle,|v\rangle$ are the neutron spin eigenstates:

$$\langle u|\vec{\sigma}.\vec{M}_\perp|u\rangle=M_{\perp z};\;\;\langle v|\vec{\sigma}.\vec{M}_\perp|v\rangle=-M_{\perp z};\;\;\langle v|\vec{\sigma}.\vec{M}_\perp|u\rangle=M_{\perp x}+iM_{\perp y};\;\;\langle u|\vec{\sigma}.\vec{M}_\perp|v\rangle=M_{\perp x}-iM_{\perp y}$$

so, sample magnetization parallel to the neutron's magnetic moment (z) does not change the neutron spin, whereas perpendicular components of magnetization 'flip' the neutron's spin

- Homework: show that for a paramagnet (where $\langle S_i^\alpha S_j^\beta\rangle=\frac{1}{3}\delta_{ij}\delta_{\alpha\beta}S(S+1)$ for spins i and j)
  - If z is parallel to **Q**, the scattering is entirely spin flip
  - If z is perpendicular to **Q**, half the scattering is spin flip

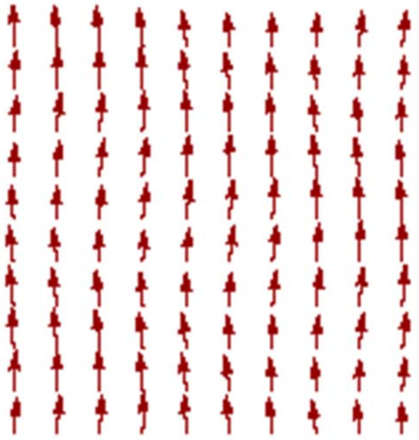
Inelastic Magnetic Scattering of Neutrons

- In the simplest case, atomic spins in a ferromagnet precess about the direction of mean magnetization

$$H = \sum_{l,l'} J(\vec{l} - \vec{l}\,')\vec{S}_l.\vec{S}_{l'} = H_0 + \sum_q \hbar\omega_q b_q^+ b_q$$

Heisenberg interaction

spin waves (magnons)

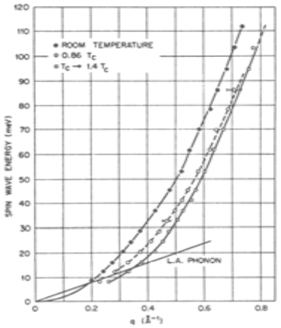


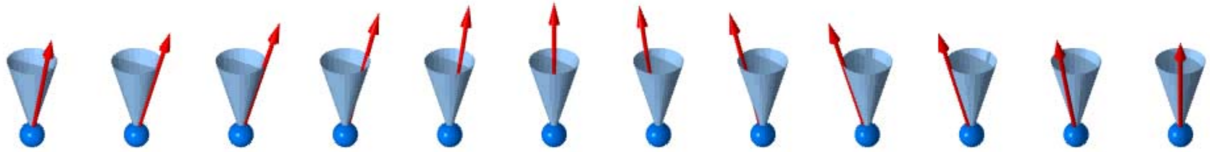
with

$$\hbar\omega_q = 2S(J_0 - J_q) \qquad \text{where} \quad J_q = \sum_l J(\vec{l}\,)e^{i\vec{q}.\vec{l}}$$

$\hbar\omega_q = Dq^2$ is the dispersion relation for a ferromagnet

Fluctuating spin is perpendicular to mean spin direction

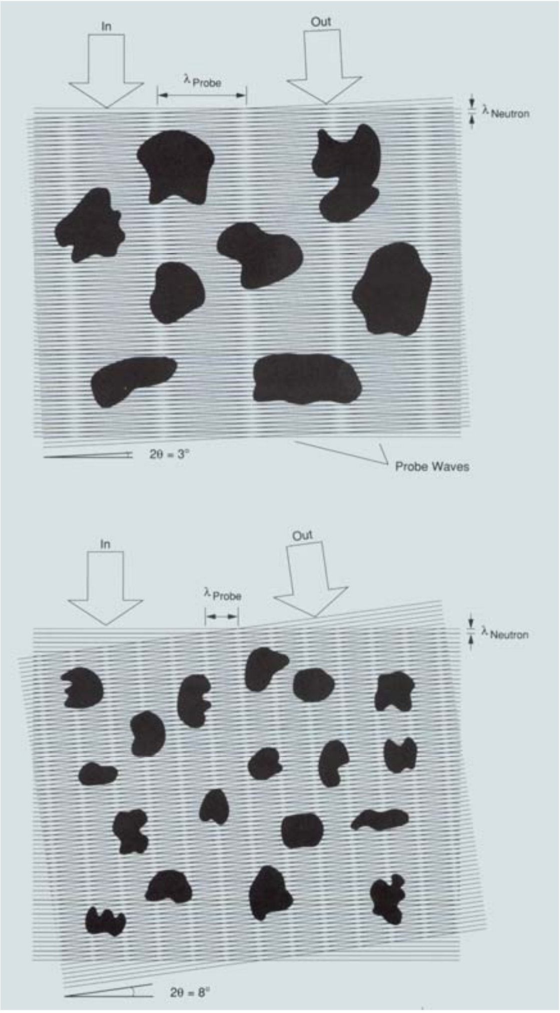




Spin wave animation courtesy of A. Zheludev (ORNL)

Diffraction

- Neutron (or x-ray) diffraction is used to measure the differential cross section, d ʃ/d∧ in the static approximation i.e. integrated over k’ – measures G(r,0)
  - Crystalline solids (elastic scattering – G(r,∞))
    - Unit cell size; crystal symmetry; atomic arrangement and thermal motions (ellipsoids)
  - Liquids and amorphous materials
  - Large scale structures



- Depending on the scattering angle, structure on different length scales, d, is measured:

$$\boxed{2\pi / Q = d = \lambda / 2\sin(\theta)}$$

- For crystalline solids & liquids, use wide angle diffraction. For large structures, e.g. polymers, colloids, micelles, etc. use small-angle scattering

Diffraction by a Lattice of Atoms

$S(\vec{Q}) = \frac{1}{N}\left\langle \sum_{i,j} e^{-i\vec{Q}.(\vec{R}_i - \vec{R}_j)} \right\rangle$ with $\vec{R}_i = \vec{i} + \vec{u}_i$ where $\vec{i}$ is the equilibrium position of atom i and $\vec{u}_i$ is any displacement (e.g. thermal) from the equilibrium position.

Ignoring thermal vibrations, S(Q) is only non-zero for Q's such that $\vec{Q}.(\vec{i} - \vec{j}) = 2M\pi$.

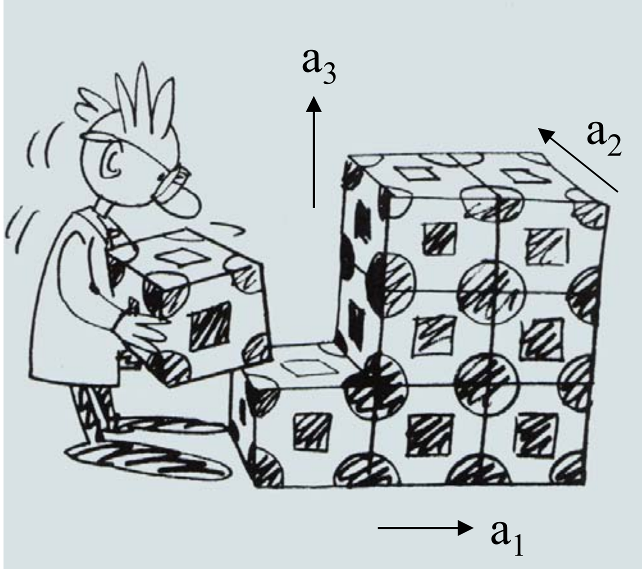
In a Bravais lattice, we can write $\vec{i} = m_{1i}\vec{a}_1 + m_{2i}\vec{a}_2 + m_{3i}\vec{a}_3$ where $\vec{a}_1, \vec{a}_2, \vec{a}_3$ are the primitive translation vectors of the unit cell.

Define $\vec{a}_1^* = \frac{2\pi}{V_0}\vec{a}_2 \wedge \vec{a}_3$ and cyclic permutations.

Then $\vec{a}_i^*.\vec{a}_j = 2\pi\delta_{ij}$.

If $\vec{Q} = \vec{G}_{hkl} = h\vec{a}_1^* + k\vec{a}_2^* + l\vec{a}_3^*$ then $\vec{Q}.(\vec{i} - \vec{j}) = 2M\pi$.

So scattering from a (frozen) lattice only occurs when the scattering wavevector, Q, is equal to a reciprocal lattice vector, G_{hkl}.



unit cell

The repeating unit of a crystal.

Direct and Reciprocal Lattices

In a Bravais lattice, we can write $\vec{R}_i = m_{1i}\vec{a}_1 + m_{2i}\vec{a}_2 + m_{3i}\vec{a}_3$ where $\vec{a}_1, \vec{a}_2, \vec{a}_3$ are the primitive translation vectors of the unit cell (see previous viewgraph).

Let's define $\vec{a}_1^* = \frac{2\pi}{V_0}\vec{a}_2 \times \vec{a}_3; \quad \vec{a}_2^* = \frac{2\pi}{V_0}\vec{a}_3 \times \vec{a}_1; \quad \vec{a}_3^* = \frac{2\pi}{V_0}\vec{a}_1 \times \vec{a}_2$

where $V_0 = \vec{\mathrm{a}}_1.(\vec{a}_2 \times \vec{a}_3)$ = the volume of the unit cell.

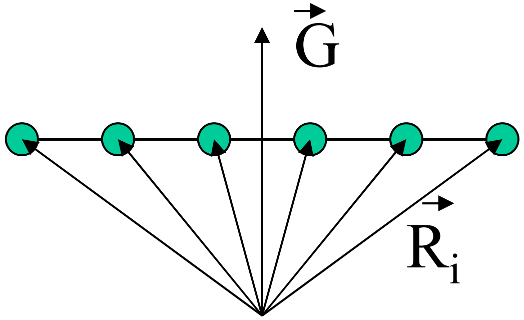
The $\vec{a}_i^*$ have the dimensions of (length)$^{-1}$ and the property that $\vec{a}_i^*.\vec{a}_j = 2\pi\delta_{ij}$, i.e. $\vec{a}_1^*$ is perpendicular to the plane defined by $\vec{a}_2$ and $\vec{a}_3$ etc.

If we choose a vector $\vec{G}_{hkl}$ defined by $\vec{G}_{hkl} = h\vec{a}_1^* + k\vec{a}_2^* + l\vec{a}_3^*$ then $\vec{G}_{hkl}.(\vec{R}_i - \vec{R}_j) = 2M\pi$.

i.e. $\vec{G}_{hkl}$ is normal to sets of planes of atoms spaced $2\pi / G_{hkl}$ apart

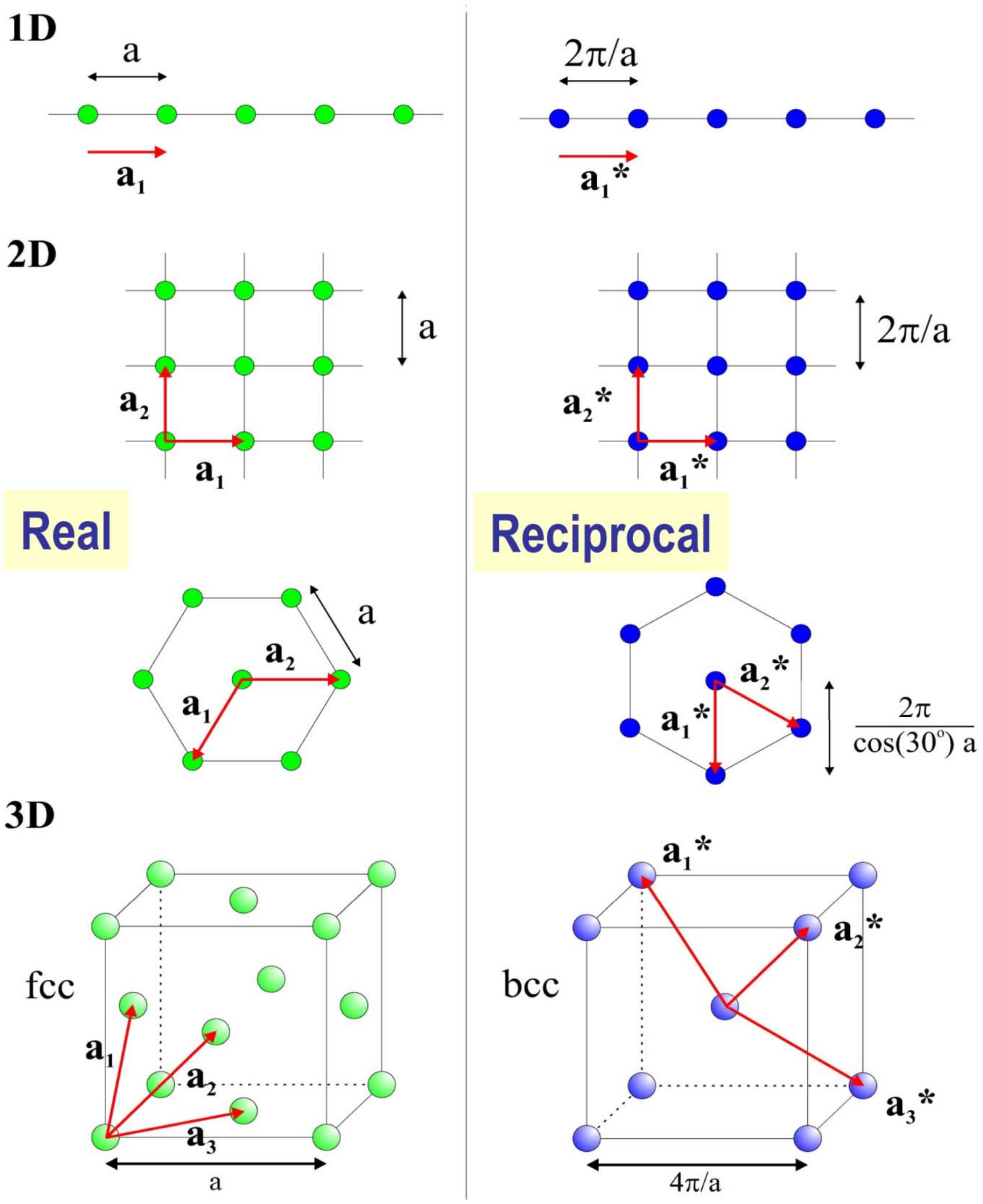
Scattering from a lattice of atoms occurs only when $\vec{Q} = \vec{G}_{hkl}$

The vectors $\vec{G}_{hkl}$ define a lattice of points called the reciprocal lattice



Homework: verify that Bragg's (λ= 2 d sinθ) follows from the above

Reciprocal Lattice:



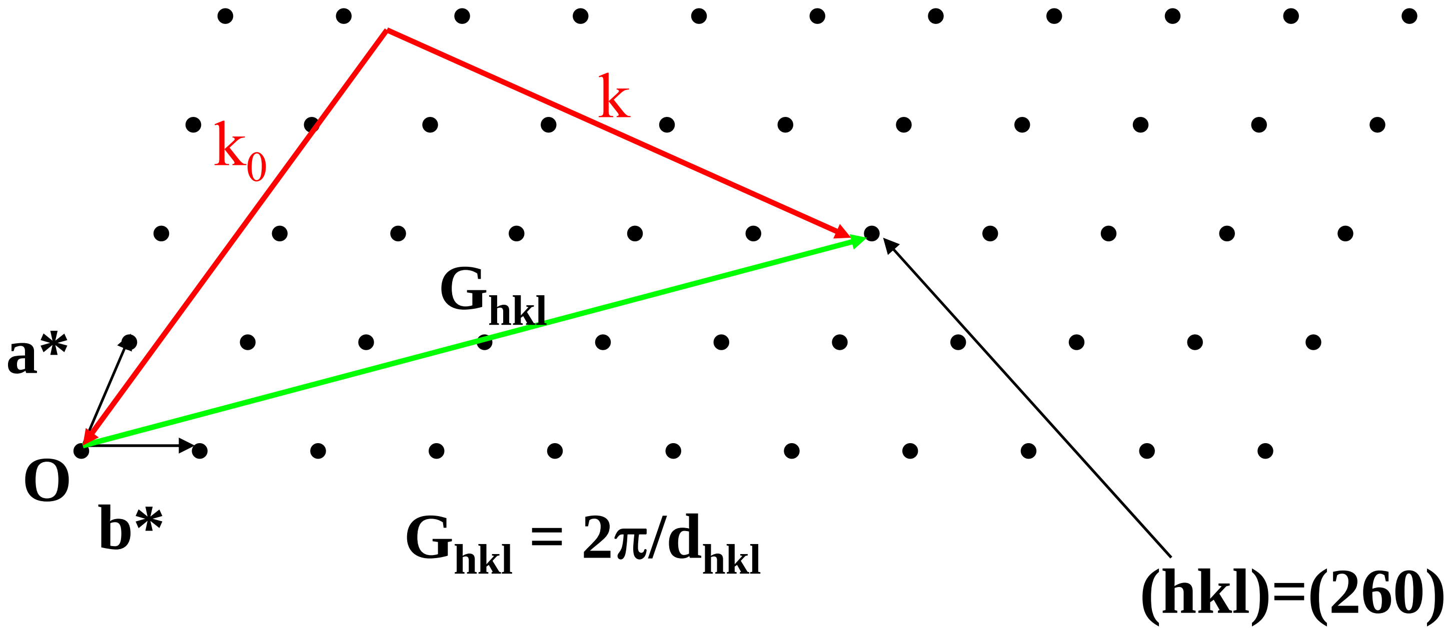
$$V_c = \vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)$$

$$\vec{a}_1^* = \frac{2\pi}{V_c} \vec{a}_2 \times \vec{a}_3$$

$$\vec{a}_2^* = \frac{2\pi}{V_c} \vec{a}_3 \times \vec{a}_1$$

$$\vec{a}_3^* = \frac{2\pi}{V_c} \vec{a}_1 \times \vec{a}_2$$

Reciprocal Space – An Array of Points (hkl) that is Precisely Related to the Crystal Lattice



$\mathbf{G_{hkl} = 2\pi/d_{hkl}}$

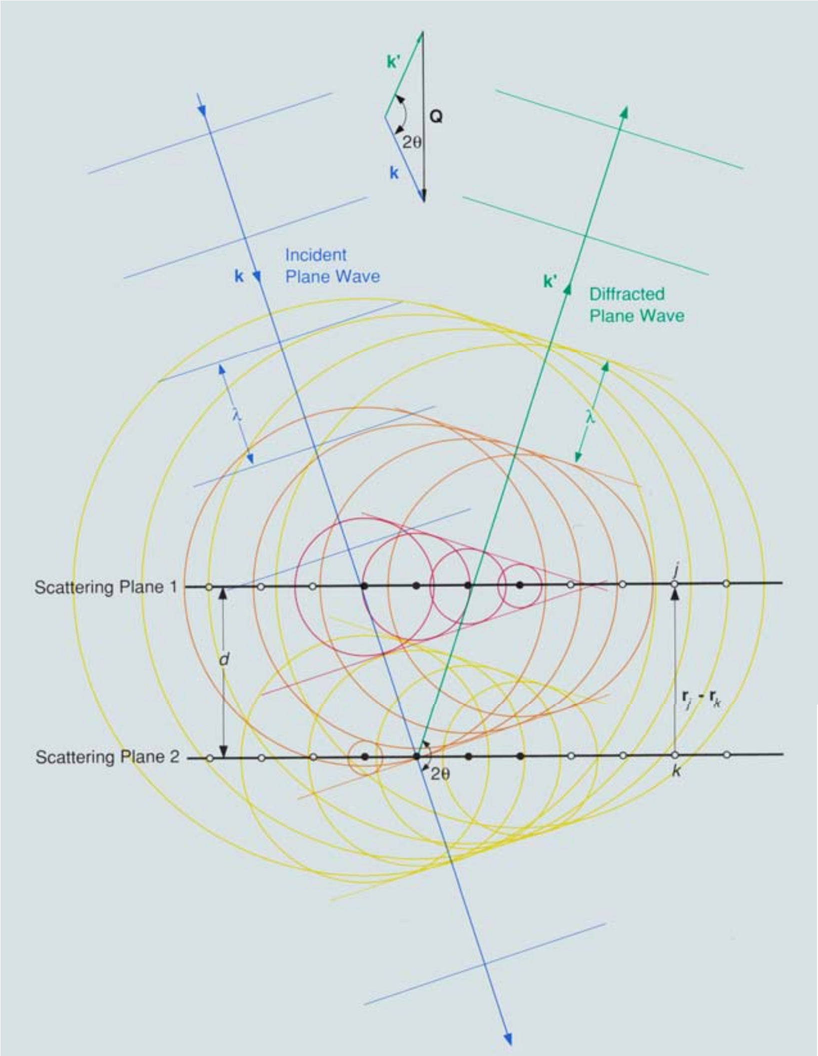
$\mathbf{a^* = 2□(b\ x\ c)/V_0}$, **etc.**

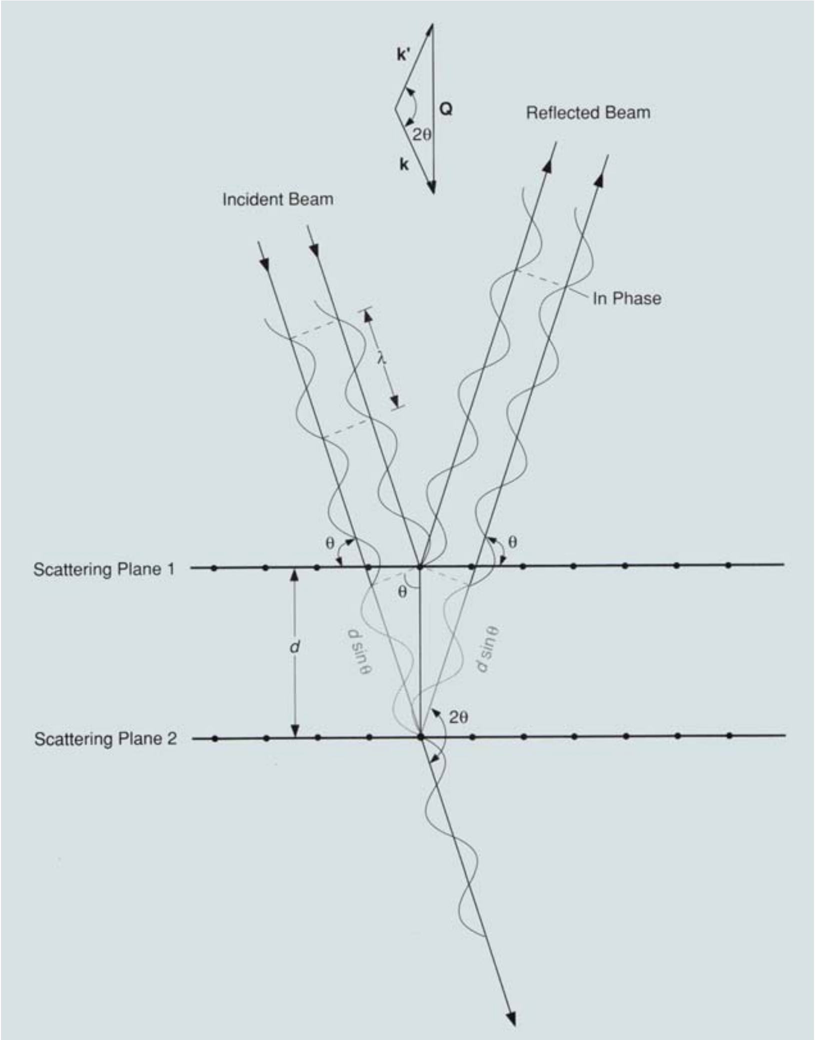
A single crystal has to be aligned precisely to record Bragg scattering

Notation

- $\vec{G}_{hkl}$ is called a reciprocal lattice vector (node denoted hkl)
- h, k and l are called Miller indices
- (hkl) describes a set of planes perpendicular to $\vec{G}_{hkl}$, separated by $2\pi/G_{hkl}$
- {hkl} represents a set of symmetry-related lattice planes
- [hkl] describes a crystallographic direction
- <hkl> describes a set of symmetry equivalent crystallographic directions

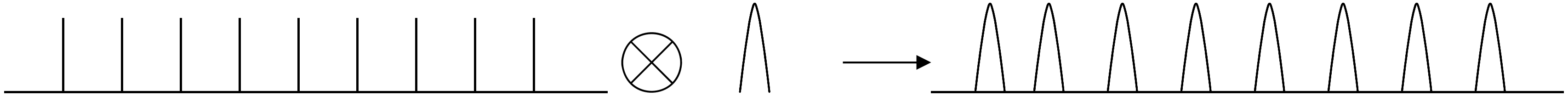
For Periodic Arrays of Nuclei, Coherent Scattering Is Reinforced Only in Specific Directions Corresponding to the Bragg Condition: $\lambda = 2\, d_{hkl} \sin(\theta)$ or $2\, k \sin(\theta) = G_{hkl}$ (where $G_{hkl} = 2\pi / d_{hkl}$)





Atomic Vibrations

- **The formalism on the previous slide works fine if the atoms are stationary: in reality, they are not**
- **Remember that** $S(\vec{Q}) = \frac{1}{N}\left\langle \sum_{i,j} e^{-i\vec{Q}.(\vec{R}_i - \vec{R}_j)} \right\rangle_{\text{ensemble}}$
- **We average over the (fluctuating) atomic positions by introducing a probability that an atom will be at given position. Instead of the Fourier Transform of ™functions, this gives the FT of the ™functions *convolved* with a spread function. The result is that S(Q) is *multiplied* by the FT of the spread function i.e. by** $\exp - Q^2 \langle u^2 \rangle / 3$ **if we use a Gaussian spread function**



- **Atomic vibrations cause a decrease in the intensity of Bragg scattering. The “missing” scattering appears between Bragg peaks and results in inelastic scattering**

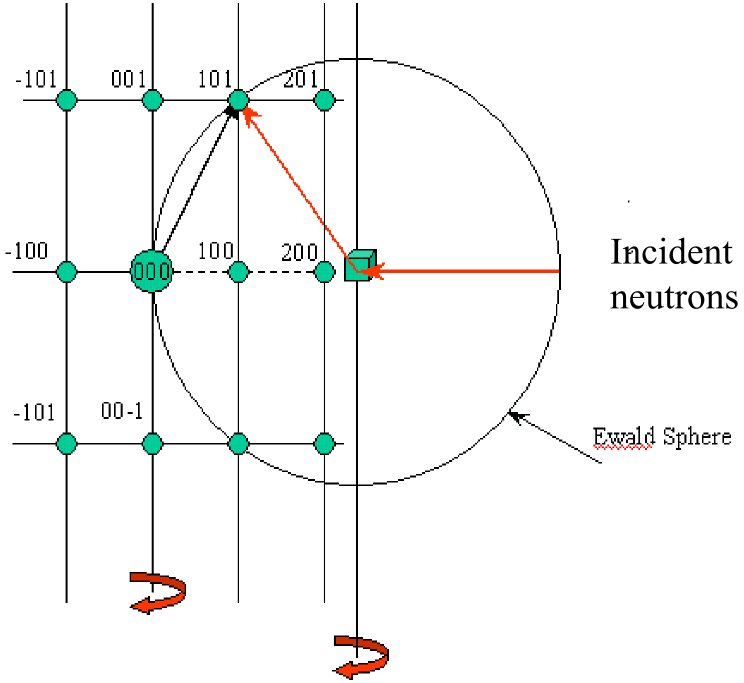
Key Points about Diffraction

- A monochromatic (single λ) neutron beam is diffracted by a single crystal only if specific geometrical conditions are fulfilled

- These conditions can be expressed in several ways:
  - Laue's conditions: $\vec{Q}.\vec{a}_1 = h; \quad \vec{Q}.\vec{a}_2 = k; \quad \vec{Q}.\vec{a}_3 = l$ with h, k, and l as integers
  - Bragg's Law: $2d_{hkl} \sin\theta = \lambda$
  - Ewald's construction

    see http://www.matter.org.uk/diffraction/geometry/default.htm

- Diffraction tells us about:
  - The dimensions of the unit cell
  - The symmetry of the crystal
  - The positions of atoms within the unit cell
  - The extent of thermal vibrations of atoms in various directions



Bragg Scattering from Crystals

Working through the math (see, for example, Squires' book), we find :

$$\left(\frac{d\sigma}{d\Omega}\right)_{Bragg} = N\frac{(2\pi)^3}{V_0}\sum_{hkl}\delta(\vec{Q}-\vec{G}_{hkl})\left|F_{hkl}(\vec{Q})\right|^2$$

where the unit - cell structure factor is given by

$$F_{hkl}(\vec{Q}) = \sum_{d}\overline{b}_d e^{i\vec{Q}.\vec{d}} e^{-W_d}$$

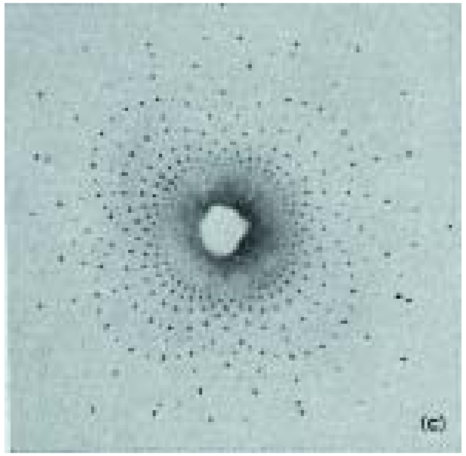
and W_d is the Debye - Waller factor that accounts for thermal motions of atoms

- Using either single crystals or powders, neutron diffraction can be used to measure F^2 (which is proportional to the intensity of a Bragg peak) for various values of (hkl).
- Direct Fourier inversion of diffraction data to yield crystal structures is not possible because we only measure the magnitude of F, and not its phase => models must be fit to the data
- Neutron powder diffraction has been particularly successful at determining structures of new materials, e.g. high T_c materials

The Structure Factor

- The intensity of scattering at reciprocal lattice points is given by the square of the structure factor $F_{hkl}(\vec{Q}) = \sum_d \overline{b}_d e^{i\vec{Q}.\vec{d}} e^{-W_d}$

- Crystallography attempts to deduce atomic positions and thermal motions from measurements of a large number of such “reflections”
  - (Reciprocal) distance between diffraction “spots” => size of unit cell
  - Systematic absences and symmetry of reciprocal lattices => crystal symmetry (e.g. bcc h+k+l=2n)
  - Intensities of “spots” => atomic positions and thermal motions



Laue diffraction pattern showing crystal symmetry

If we could measure the complex quantity F_{hkl} we could figure out the positions of all atoms. But we only measure $| F_{hkl} |^2$. In fact, we would be better off if diffraction measured phase of scattering rather than amplitude! Unfortunately, nature did not oblige us.

The Phase Problem

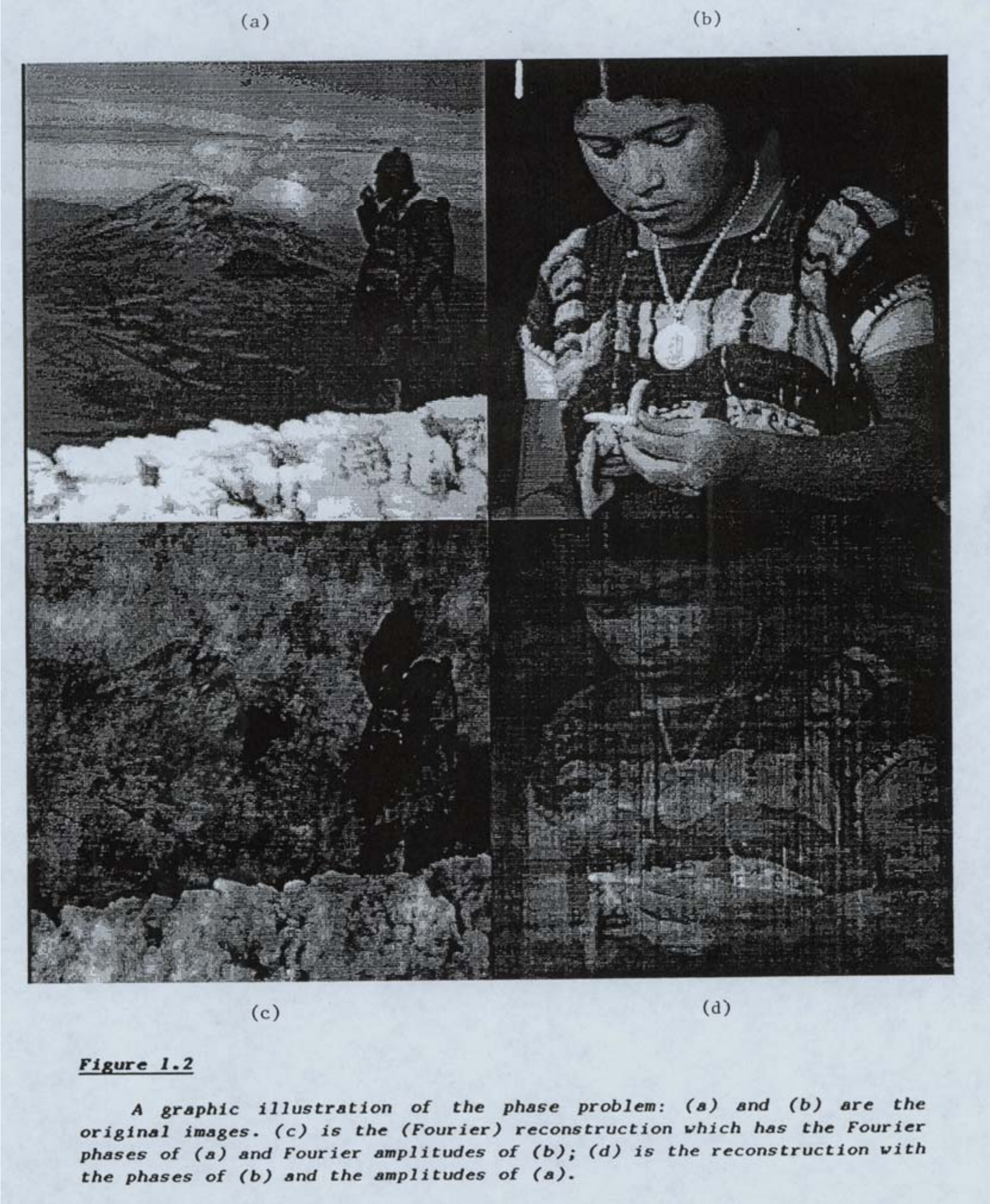
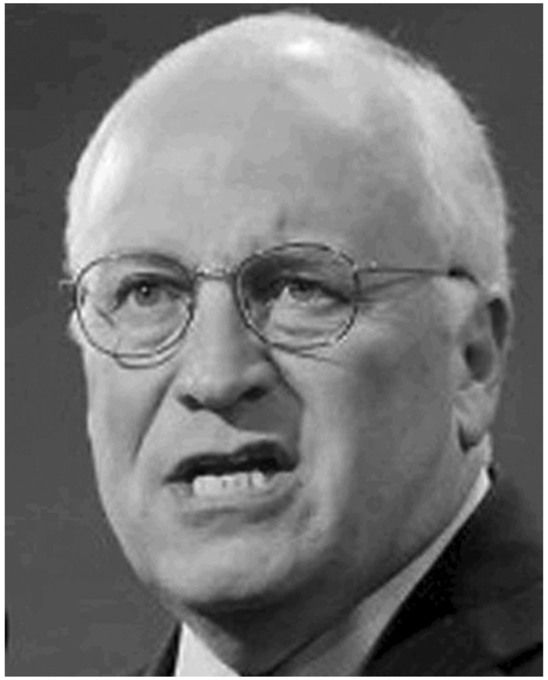


Figure 1.2

A graphic illustration of the phase problem: (a) and (b) are the original images. (c) is the (Fourier) reconstruction which has the Fourier phases of (a) and Fourier amplitudes of (b); (d) is the reconstruction with the phases of (b) and the amplitudes of (a).

Picture by courtesy of D. Sivia

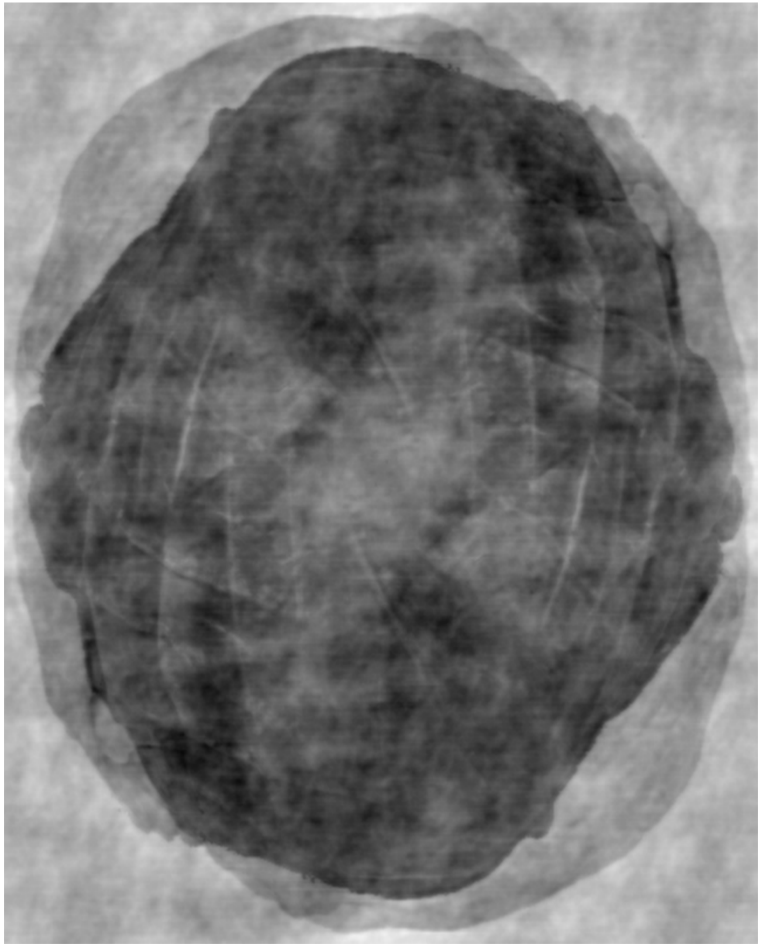
Object A



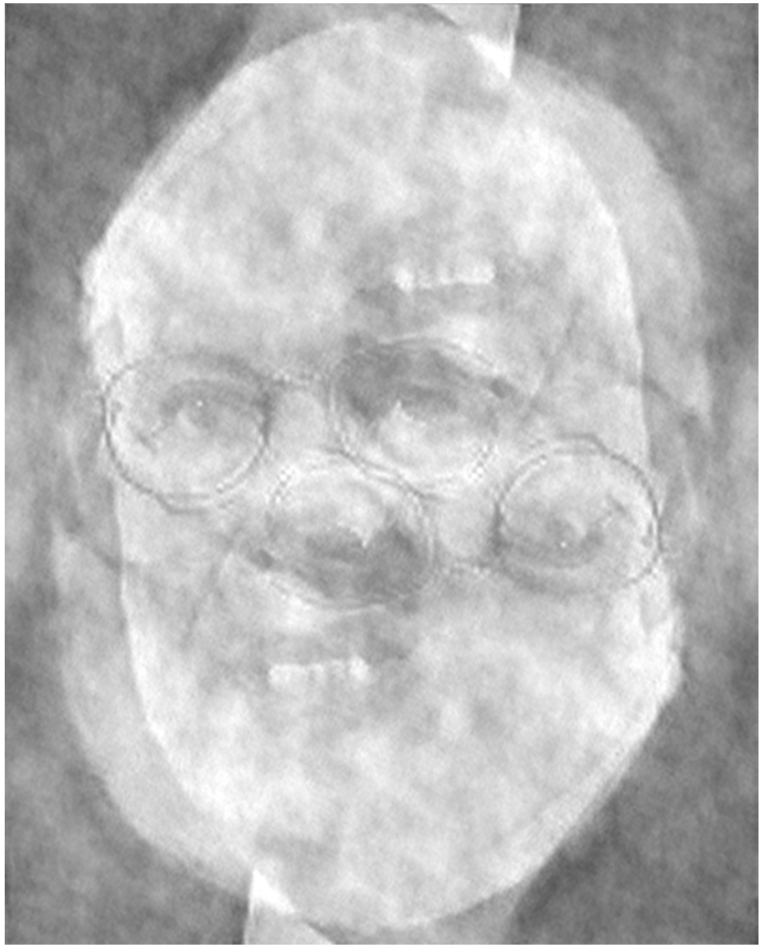
Object B

Professor Sinha's demonstration of the "Phase Problem" is much more memorable

Fourier Reconstruction with phases of object A and amplitudes of Object B

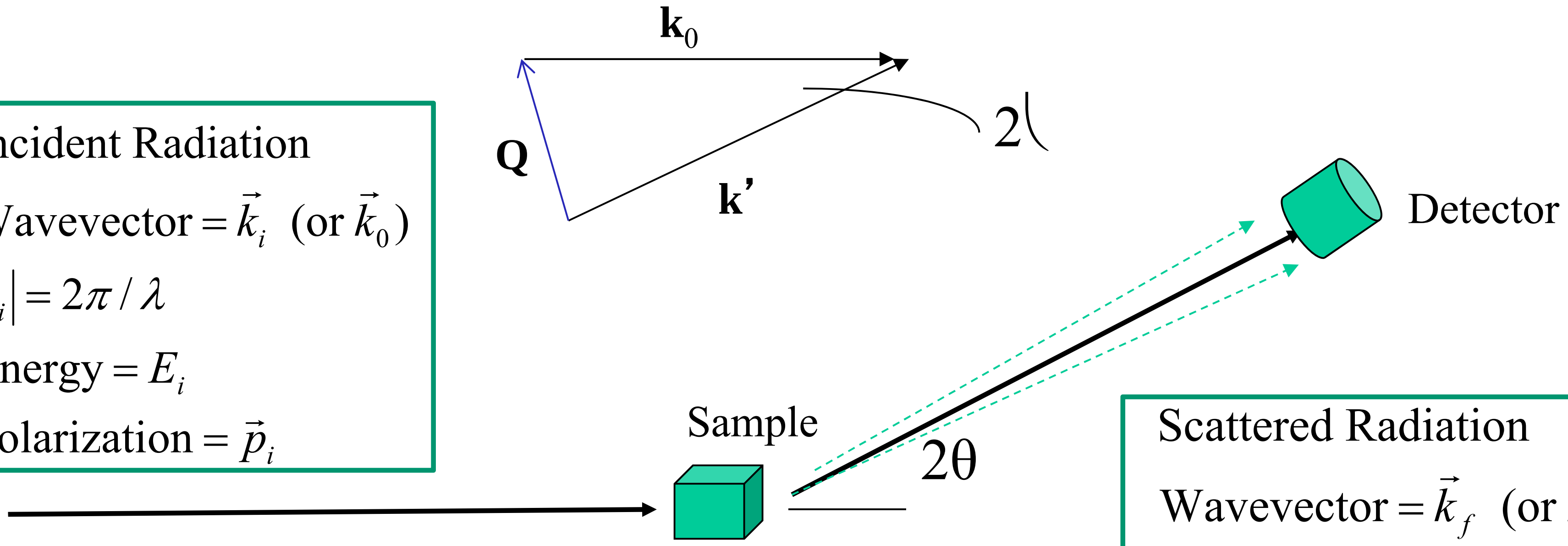


Fourier Reconstruction with phases of object B and amplitudes of Object A



PHASE tells us where the different parts of the object are located!

Now that we know what the scattering cross section means, how do we measure it?



Incident Radiation

Wavevector $= \vec{k}_i$ (or $\vec{k}_0$)

$|k_i| = 2\pi / \lambda$

Energy $= E_i$

Polarization $= \vec{p}_i$

Scattered Radiation

Wavevector $= \vec{k}_f$ (or $\vec{k}'$)

Energy $= E_f$

Polarization $= \vec{p}_f$

Wavevector Transfer, $\vec{Q} = \vec{k}_f - \vec{k}_i$

Energy Transfer, $\Delta E = h\upsilon = \hbar\omega = E_f - E_i$

For x-rays: $\Delta E << E_f$ or E_i so $Q = 2k_i \sin\theta$

Polarization, $\vec{p}_i \rightarrow \vec{p}_f$

Notice that the finite size of the detector and sample imply uncertainty in the direction of the wavevectors

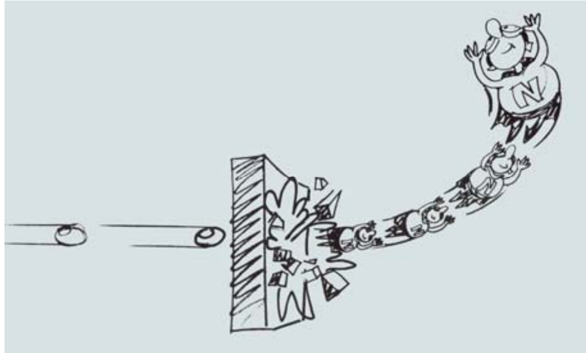
Specifying the magnitude of the wavevector: CW or TOF?

- Two types of neutron source: continuous and pulsed

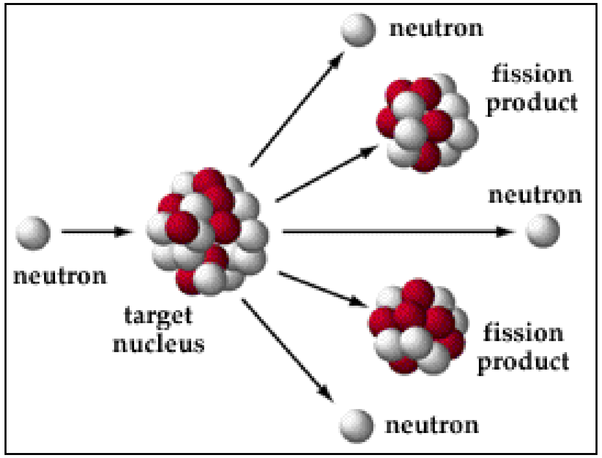
- Two (principal) methods of making neutrons: fission & spallation

- The magnitude of a neutron wavevector (i.e. the neutron velocity) can be specified in two ways:
  - Using Bragg scattering from a single crystal (or an array of crystals)
  - Using time-of-flight for a pulsed beam

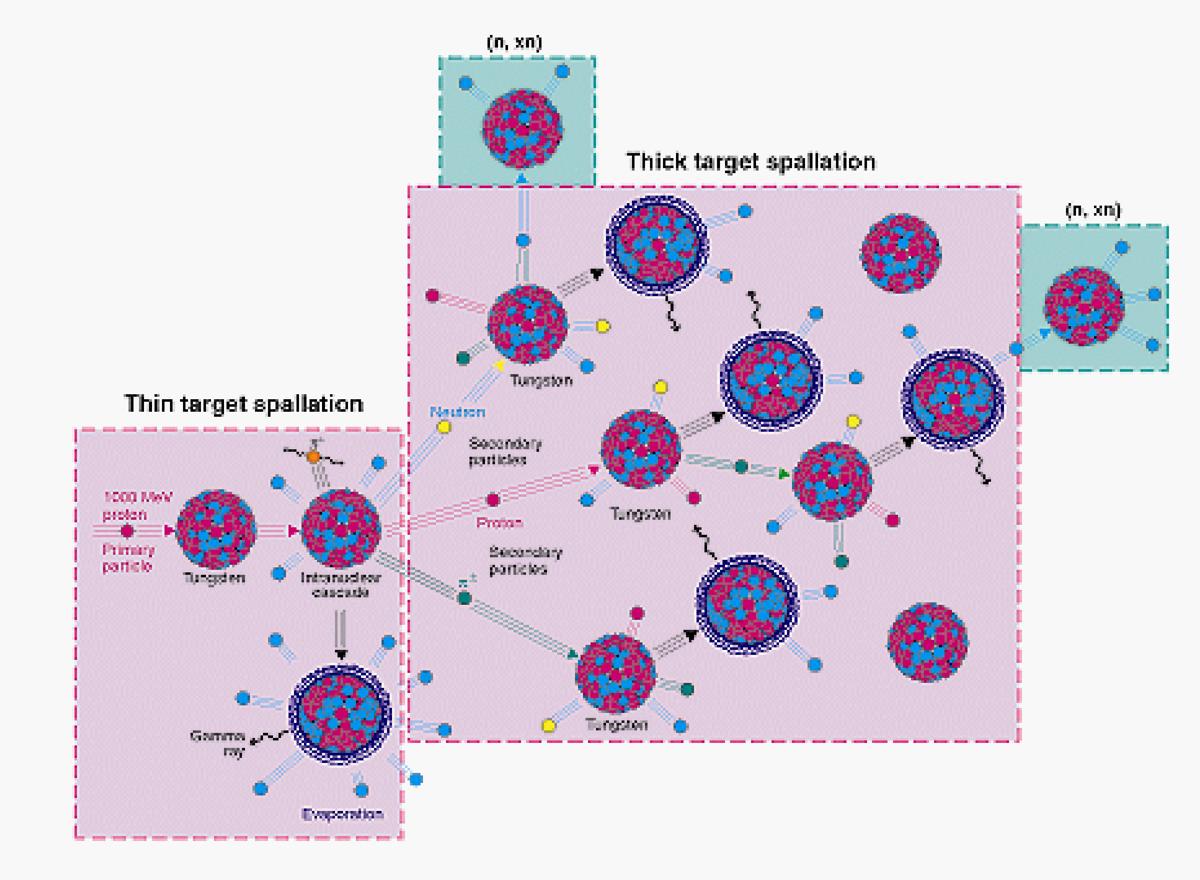
Nuclear Fission & Spallation are the Methods of Choice to Produce Neutrons for Scattering



Artist's view of spallation



Nuclear Fission



Spallation

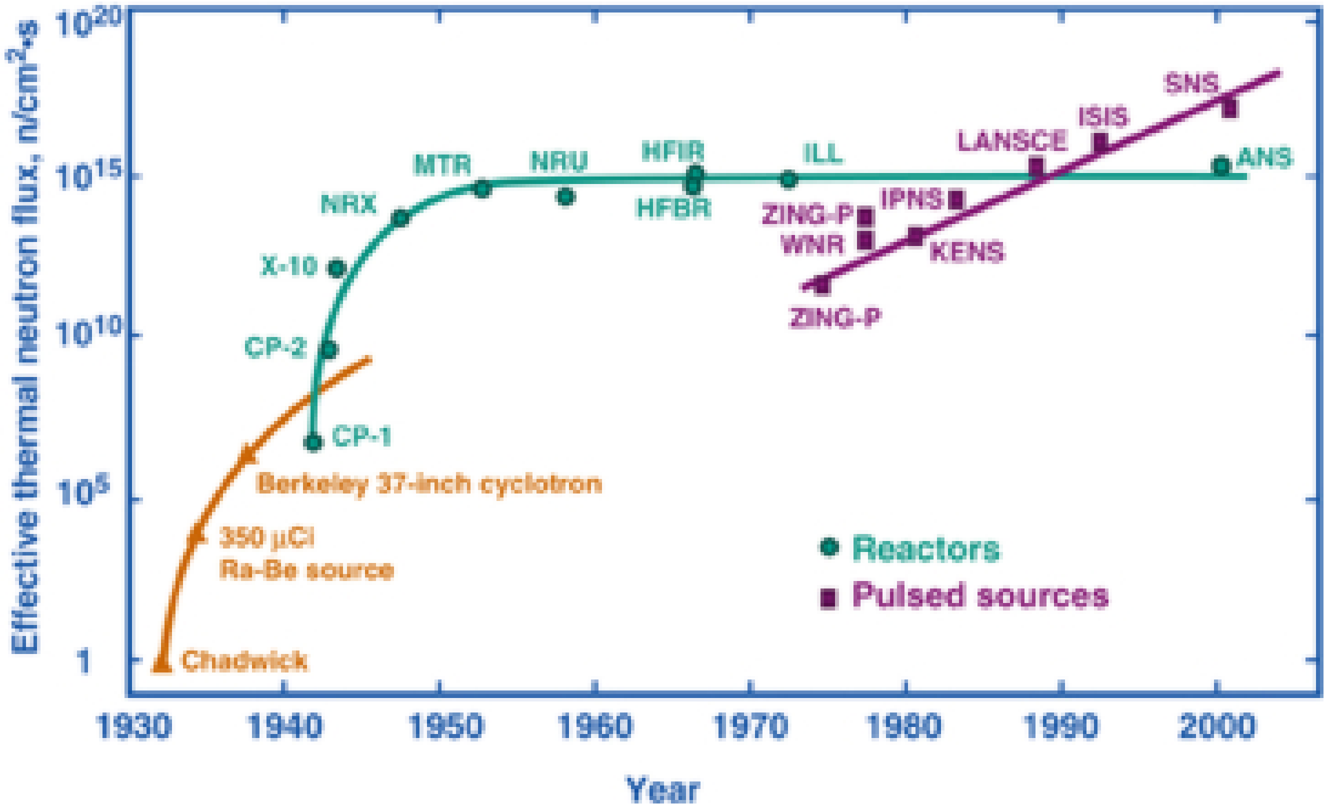
The Energy Cost of Various Neutron Sources

- For high-power sources the driving issue is heat removal => use spallation for high power sources
  - ~ 190 MeV per neutron for fission
  - ~ 25 MeV per neutron for spallation with protons (threshold at E_p~ 120 MeV)
  - ~ 1500 MeV per neutron for (n,p) on Be using 13 MeV protons
  - ~ 3000 MeV per neutron for electrons

- Driving issue for low-intensity sources is cost (electric power, regulatory, manpower etc)
  - Cost has to be kept “low” (i.e. construction ~$10-20M)
  - Cost/benefit is still the metric
  - Spallation and fission cost too much (absent a “killer app” money maker)
  - Use Be (p,n) or electrons on Ta

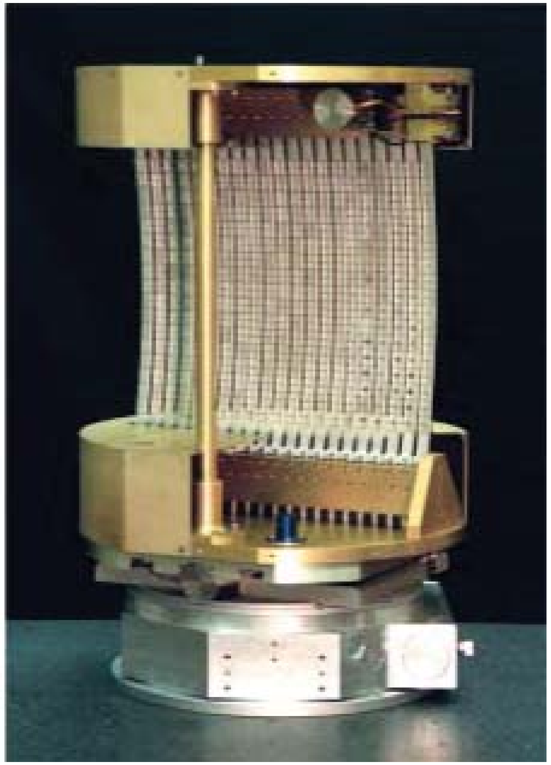
Relative Performance of CW and pulsed neutron sources

- Be very careful…..



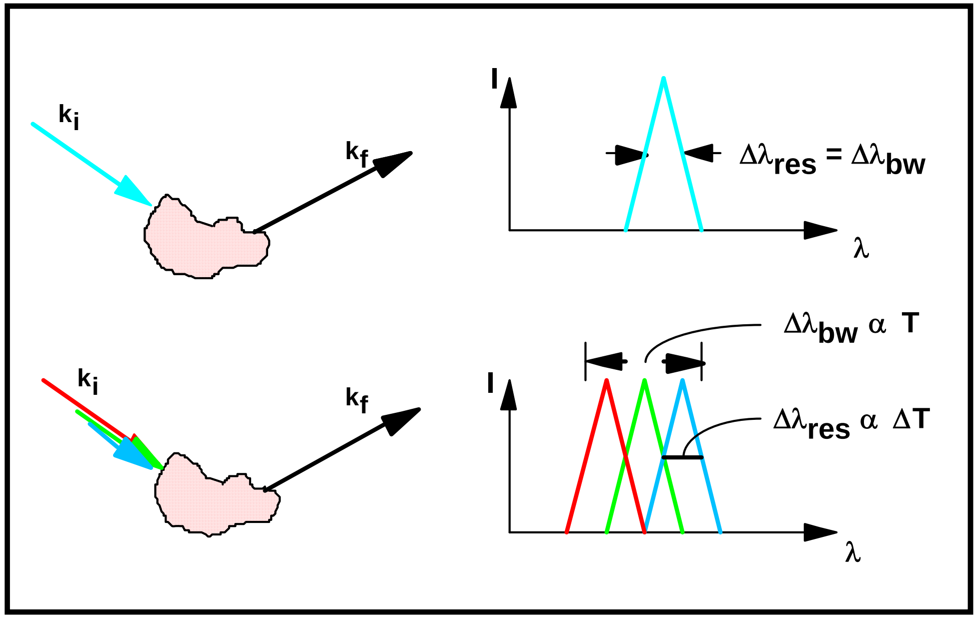
Neutron Monochromators

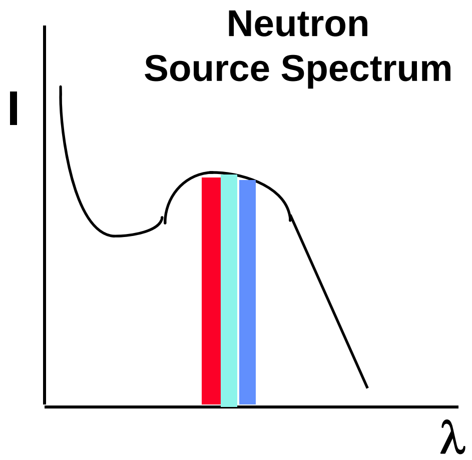
A simple, vertically focusing monochromator produced by Riso National Lab in Denmark comprised of 15 single crystals



A vertical and horizontally focusing monochromator fabricated by a Johns Hopkins team for the NCNR.

Simultaneously Using Neutrons With Many Different Wavelengths Enhances the Efficiency of Neutron Scattering Experiments

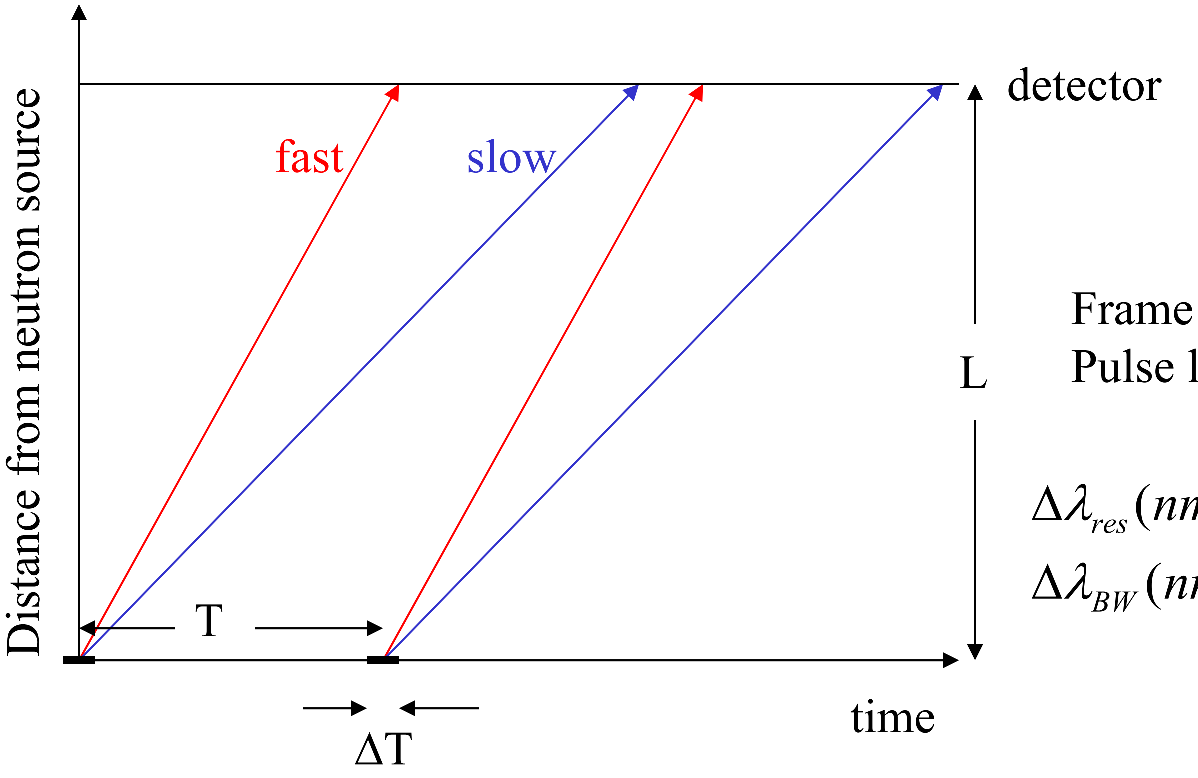




Potential Performance Gain relative to use of a Single Wavelength is the Number of Different Wavelength Slices used

Time of Flight

- At pulsed neutron sources (or with a chopped beam at a reactor), the neutron's TOF is used to determine it's speed (and, hence, wavelength)
- For elastic scattering (diffraction, SANS, reflectometry) no neutron monochromatization is needed

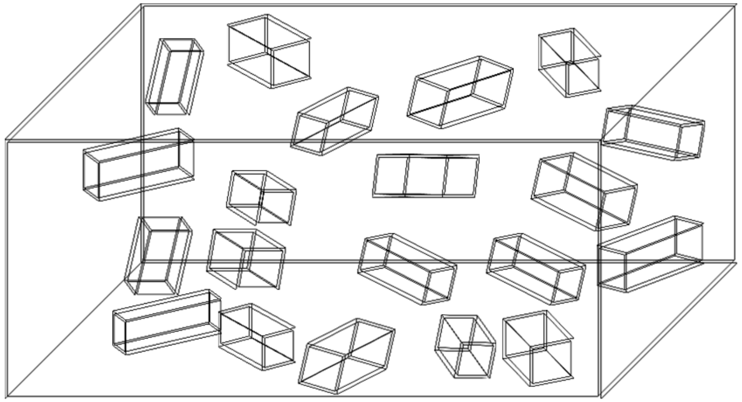


Frame length, T
Pulse length, ΔT

$$\Delta\lambda_{res}(nm) \approx 0.4\Delta T(ms) / L(m)$$

$$\Delta\lambda_{BW}(nm) \approx 0.4T(ms) / L(m)$$

Powder – A Polycrystalline Mass



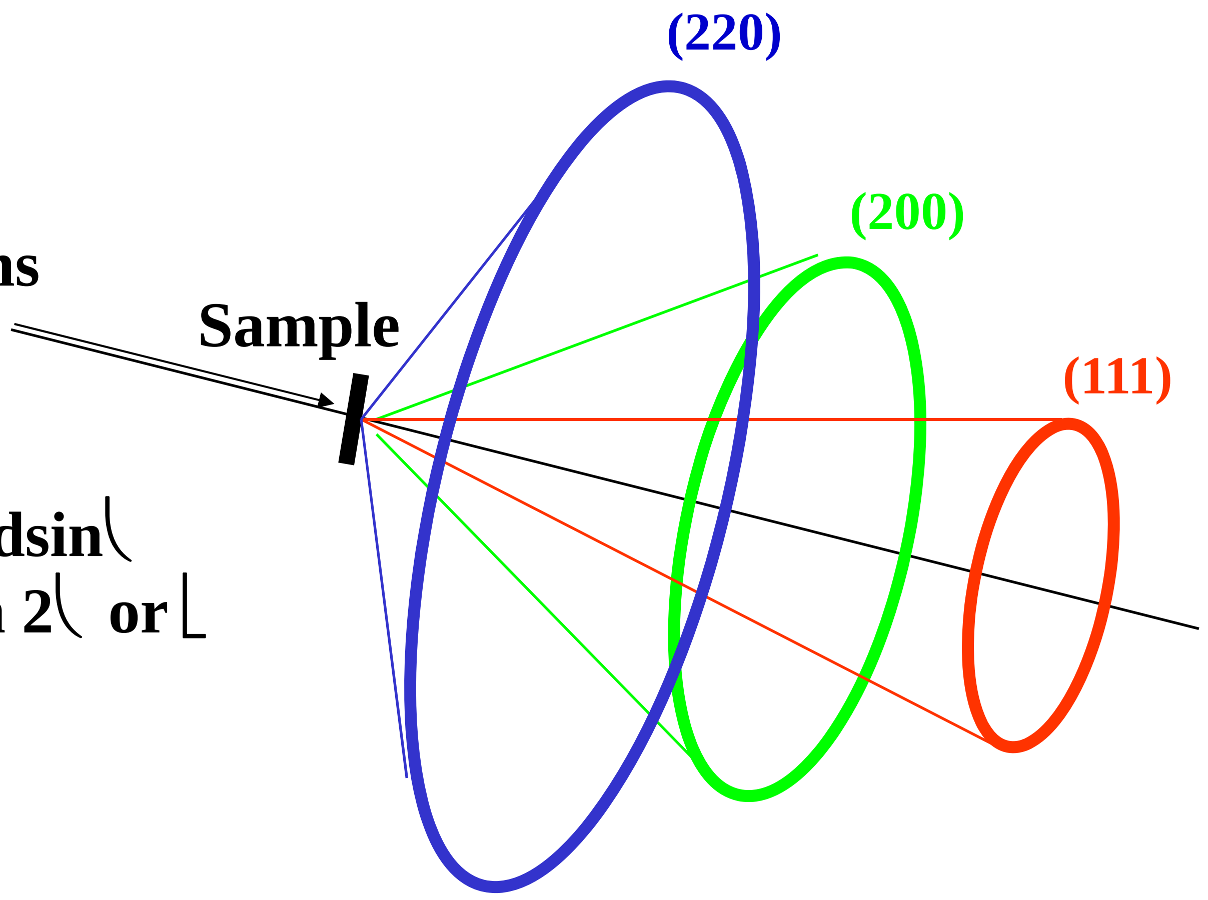
All orientations of crystallites possible

Typical Sample: 1cc powder of
10μm crystallites - 10^9 particles
if 1μm crystallites - 10^{12} particles

Single crystal reciprocal lattice
- smeared into spherical shells

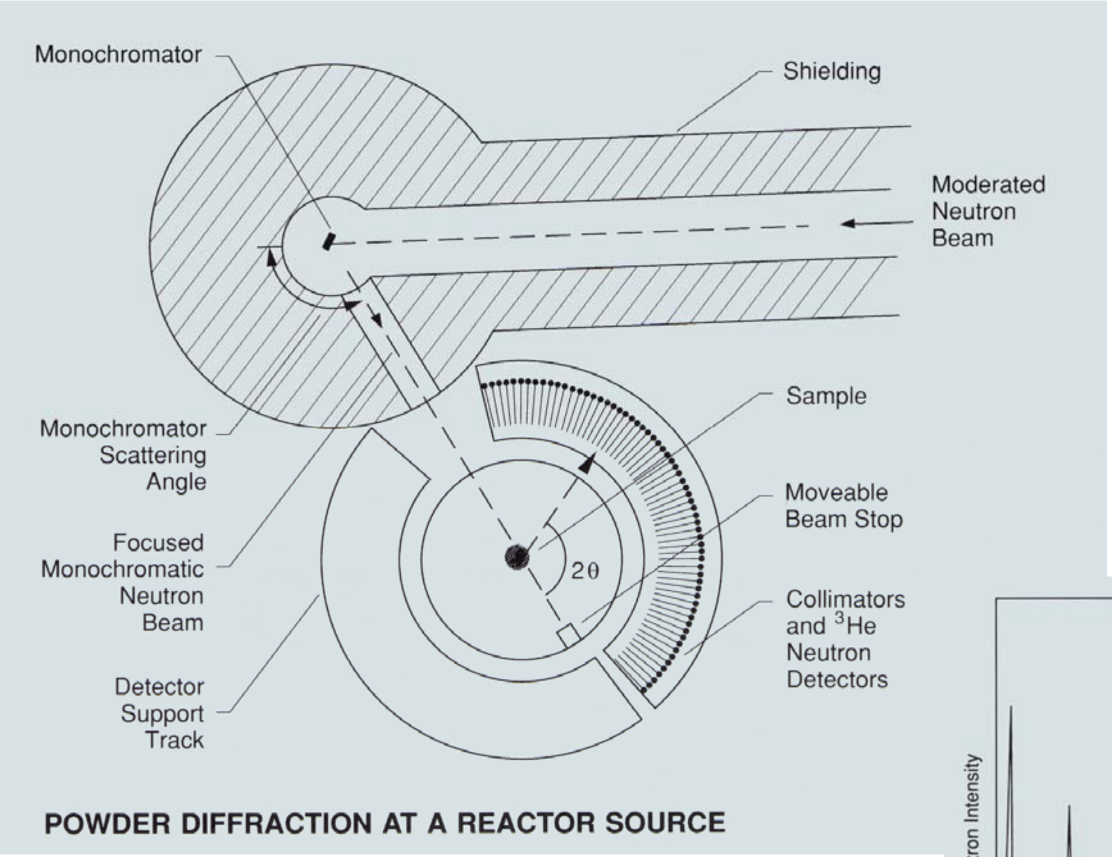
Powder Diffraction gives Scattering on Debye-Scherrer Cones

Incident beam
x-rays or neutrons



Bragg's Law $\lambda = 2d\sin\theta$
Powder pattern – scan 2θ or λ

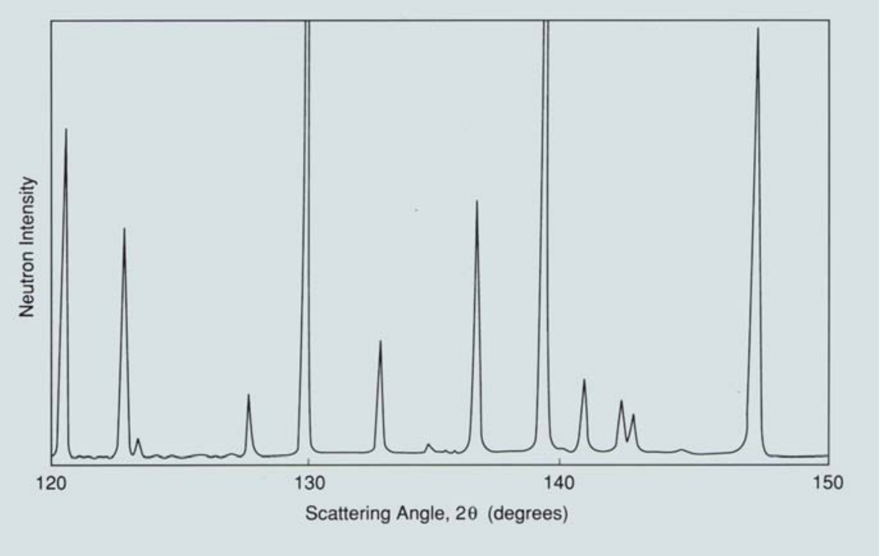
Measuring Neutron Diffraction Patterns with a Monochromatic Neutron Beam



POWDER DIFFRACTION AT A REACTOR SOURCE

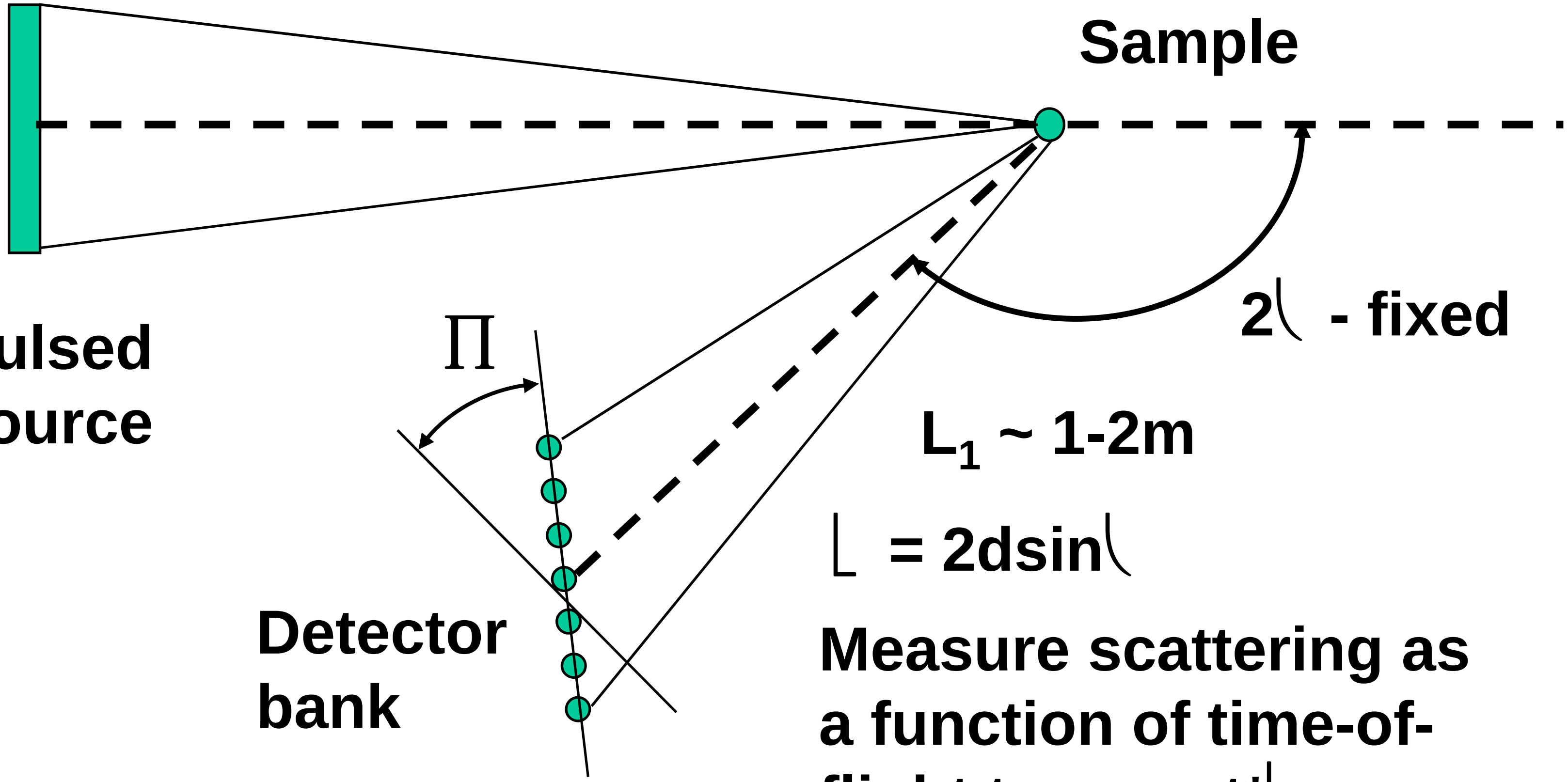
Use a continuous beam of mono-energetic neutrons.

Since we know the neutron wavevector, k, the scattering angle gives G_{hkl} directly: $G_{hkl} = 2\,k \sin\theta$



A POWDER DIFFRACTION PATTERN RECORDED AT A REACTOR

Neutron Powder Diffraction using Time-of-Flight



L_o= 9-100m

Sample

Pulsed source

Π

2θ - fixed

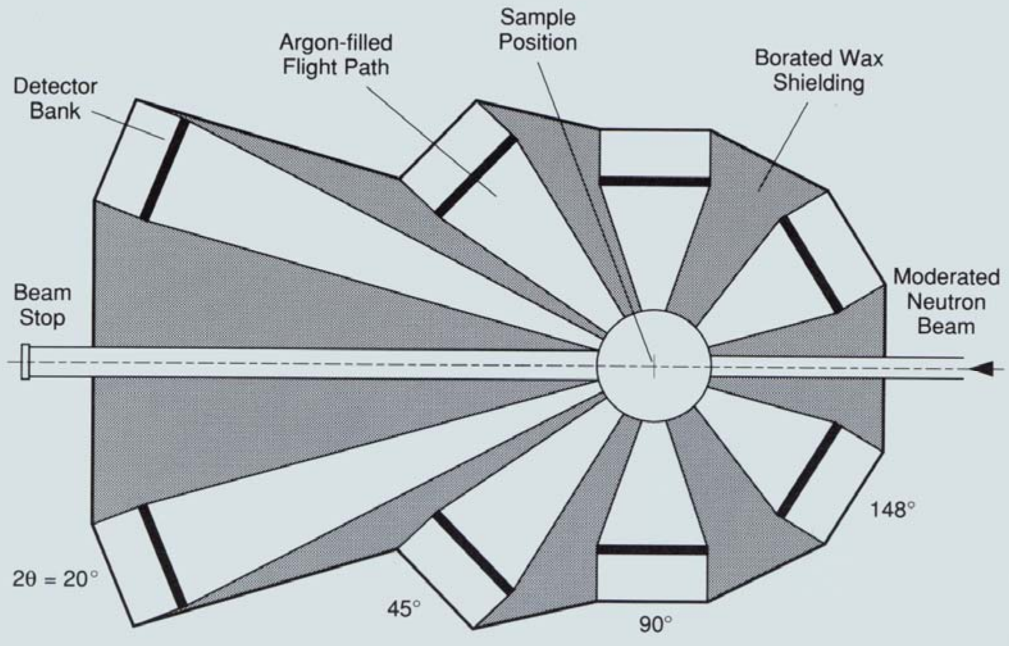
L_1 ~ 1-2m

Detector bank

$\lambda = 2d\sin\theta$

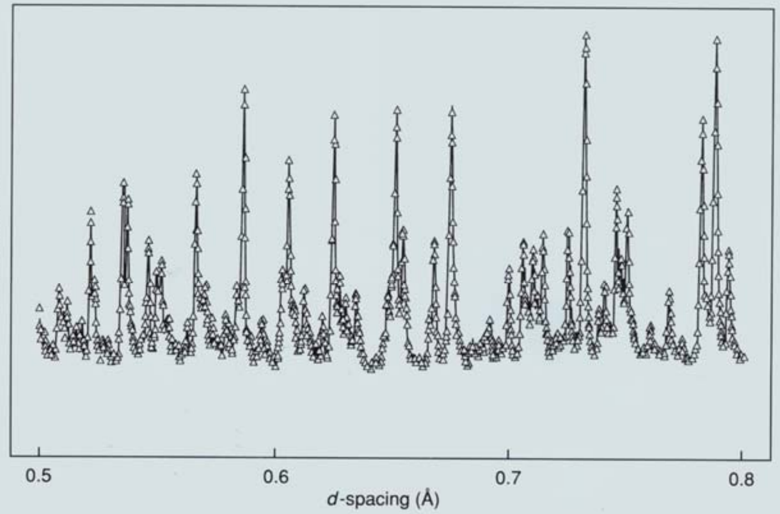
Measure scattering as a function of time-of-flight t = const*λ

Time-of-Flight Powder Diffraction



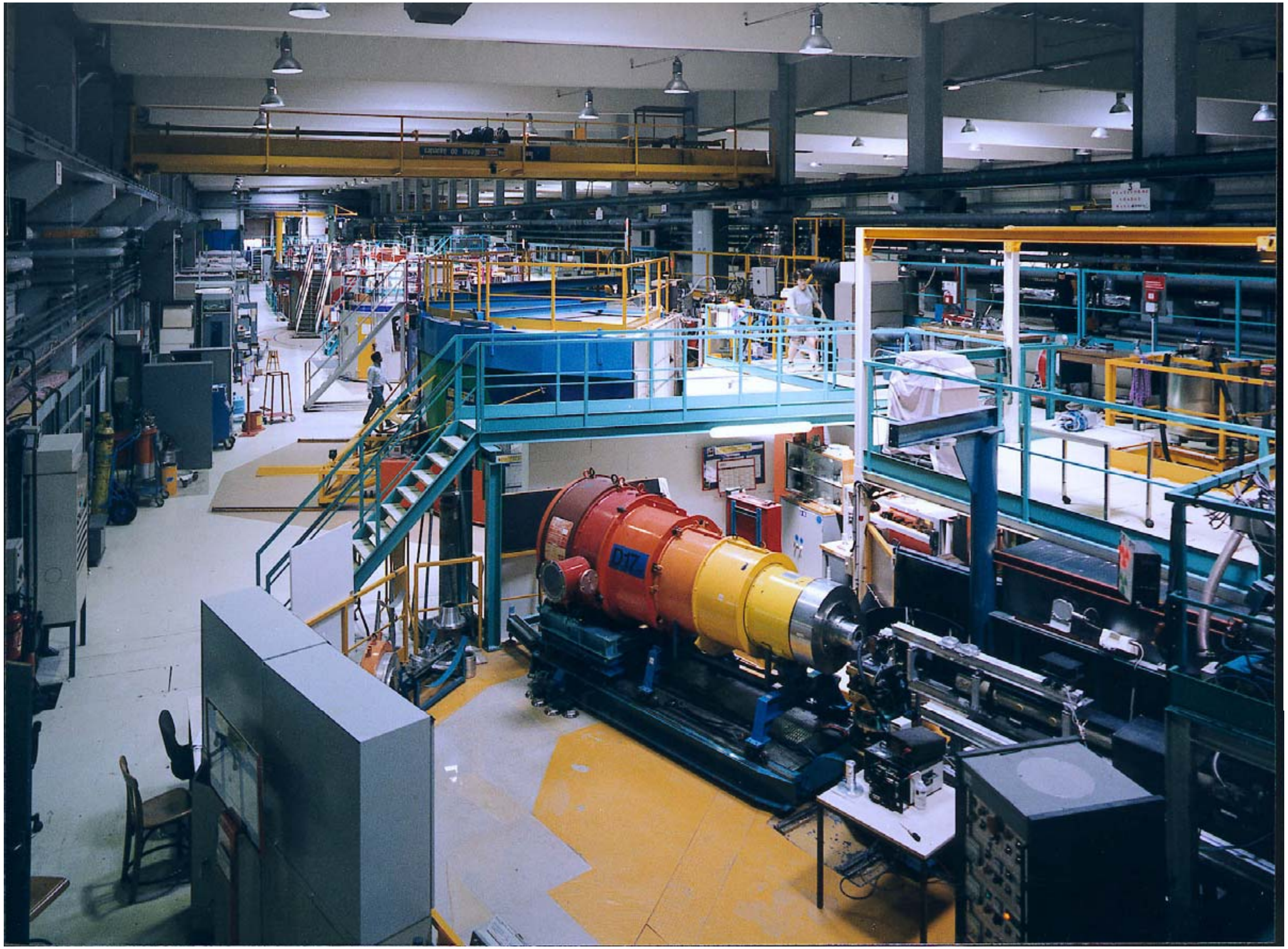
POWDER DIFFRACTION AT A SPALLATION SOURCE

Use a pulsed beam with a broad spectrum of neutron energies and separate different energies (velocities) by time of flight.



A POWDER DIFFRACTION PATTERN RECORDED AT A SPALLATION SOURCE

A ~ 30 X 20 m^2 Hall at the ILL Houses About 30 Spectrometers of different shapes and colors



Brightness & Fluxes for Neutron & X-Ray Sources

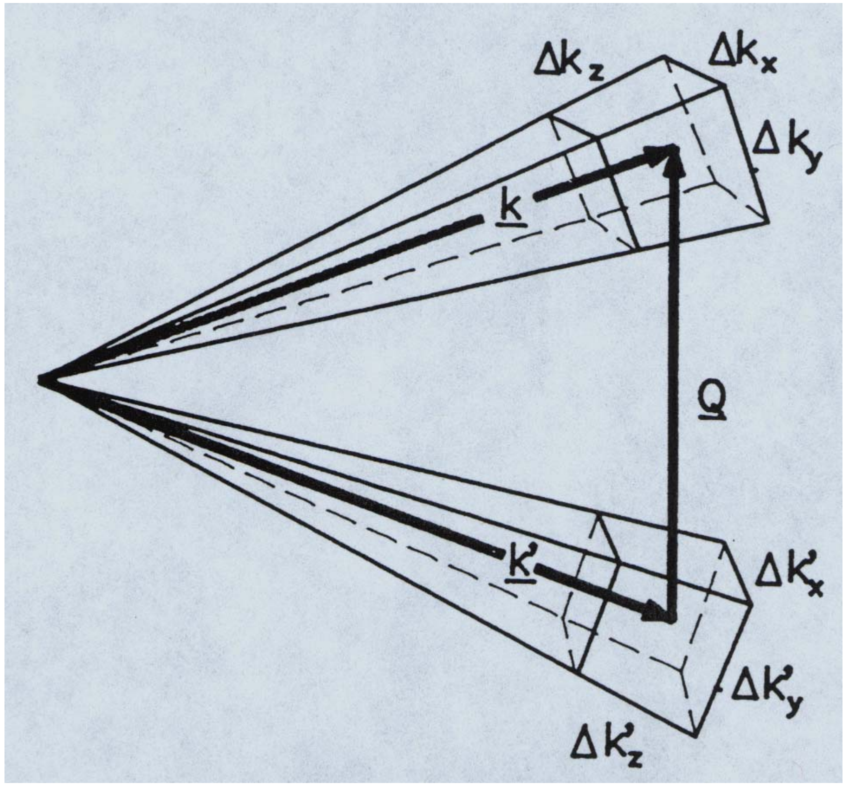
	Brightness *(s^{-1} m^{-2} $ster^{-1}$)*	*dE/E* *(%)*	*Divergence* *($mrad^2$)*	*Flux* *(s^{-1} m^{-2})*
Neutrons	10^{15}	2	10 x 10	10^{11}
Rotating Anode	10^{16}	3	0.5 x 10	5×10^{10}
Bending Magnet	10^{24}	0.01	0.1 x 5	5×10^{17}
Wiggler	10^{26}	0.01	0.1 x 1	10^{19}
Undulator (APS)	10^{33}	0.01	0.01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

Flux = brightness * divergence; brilliance = brightness / energy bandwidth

Why are there so many types of neutron instrument?

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

- When the box-like resolution volumes in the figure are convolved, the overall resolution width is the quadrature sum of the box sizes. Small “boxes” give good resolution.

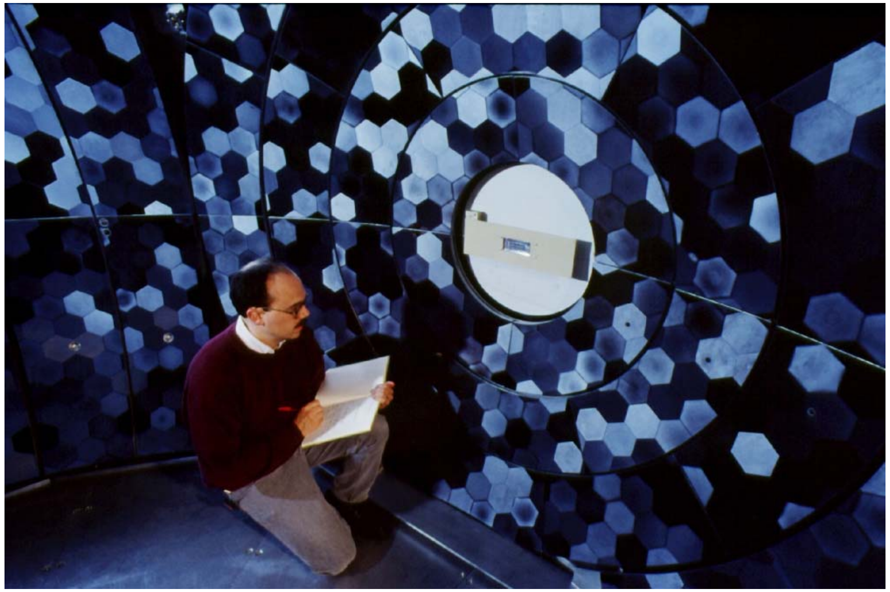


- The total signal in a scattering experiment is proportional to the product of the “box” sizes

The better the resolution, the lower the count rate

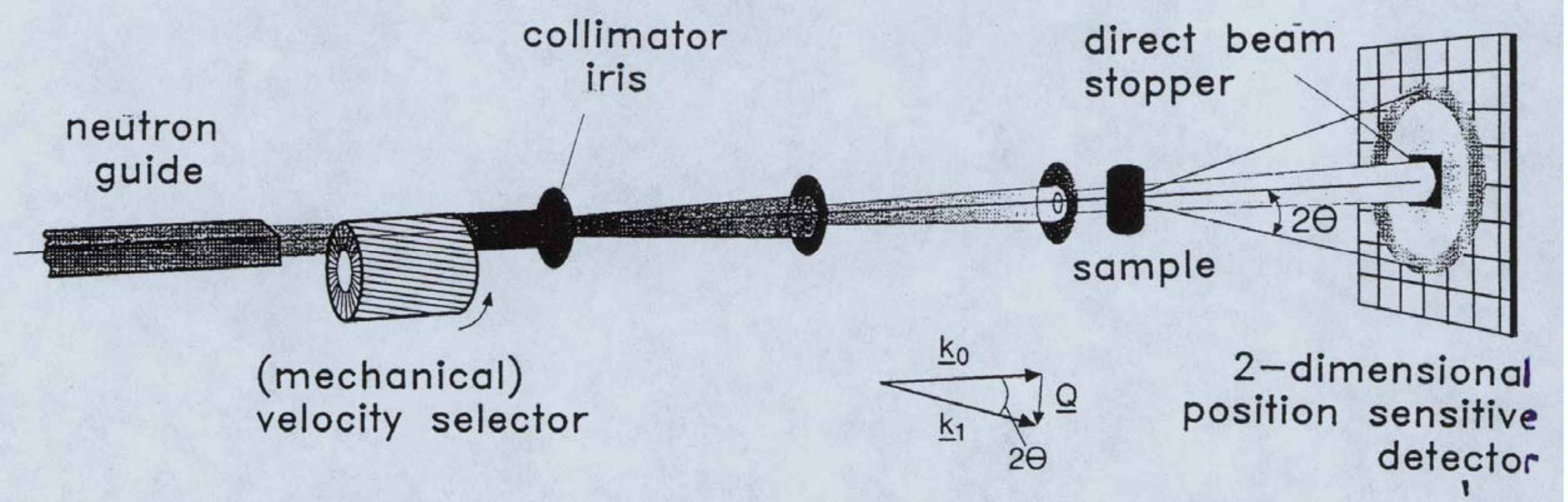
Examples of Specialization of Spectrometers: Optimizing the Signal for the Science

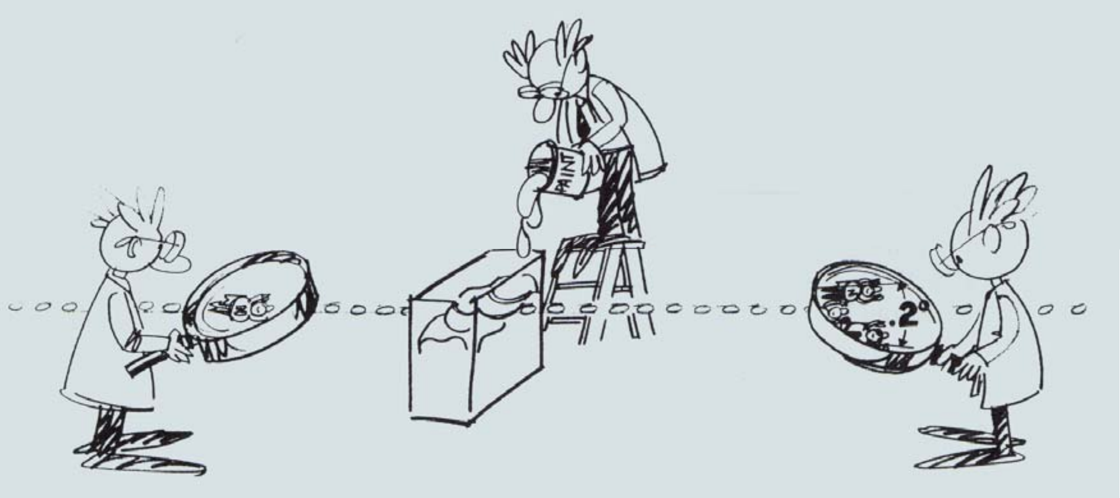
- Small angle scattering [$Q = 4\pi \sin\theta/\lambda$; $(\delta Q/Q)^2 = (\Delta\lambda/\lambda)^2 + (\cot\theta\, d\theta)^2$]
  - Small diffraction angles to observe large objects => long (20 m) instrument
  - poor monochromatization ($\Delta\lambda/\lambda \sim 10\%$) sufficient to match obtainable angular resolution (1 cm^2 pixels on 1 m^2 detector at 10 m => $\Delta\theta \sim 10^{-3}$ at $\theta \sim 10^{-2}$))
- Back scattering [$\theta = \pi/2$; $\lambda = 2 d \sin\theta$; $\Delta\lambda/\lambda = \cot\theta + \ldots$]
  - very good energy resolution (~neV) => perfect crystal analyzer at $\theta \sim \pi/2$
  - poor Q resolution => analyzer crystal is very large (several m^2)



The NIST 30m SANS Instrument Under Construction

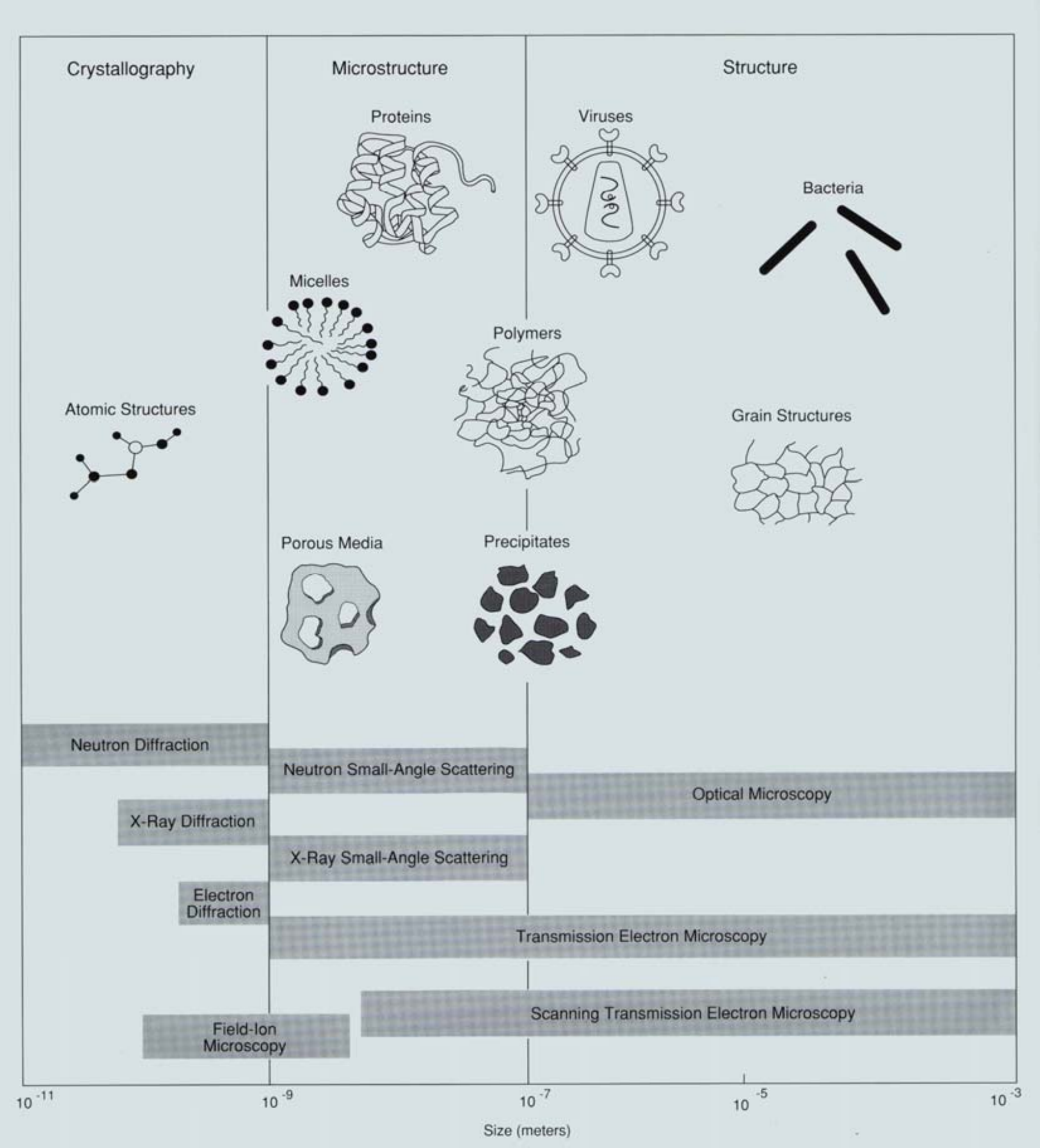
Two Views of the Components of a Typical Reactor-based SANS Diffractometer





Note that SANS, like other diffraction methods, probes material structure in the direction of (vector) $\vec{Q}$

Where Does SANS Fit As a Structural Probe?



- SANS resolves structures on length scales of 1 – 1000 nm
- Neutrons can be used with bulk samples (1-2 mm thick)
- SANS is sensitive to light elements such as H, C & N
- SANS is sensitive to isotopes such as H and D

The Fermi Pseudo-Potential for Neutrons

$$\frac{d\sigma}{d\Omega}=\frac{1}{\Phi}\frac{1}{d\Omega}\sum_{\vec{k}'\text{ in d}\Omega}W_{\vec{k}\to\vec{k}'}$$ where the sum is over probabilities of all transitions

By Fermi's Golden Rule : $$\sum_{\vec{k}'\text{ in d}\Omega}W_{\vec{k}\to\vec{k}'}=\frac{2\pi}{\hbar}\rho_{\vec{k}'}\left|\left\langle\vec{k}'\middle|V\middle|\vec{k}\right\rangle\right|^2=\frac{2\pi}{\hbar}\rho_{\vec{k}'}\frac{1}{Y^2}\left|\int_Y V(\vec{r})e^{i(\vec{k}-\vec{k}').\vec{r}}d\vec{r}\right|^2$$

where $\rho_{\vec{k}'}$ is # of momentum states in dΩ, per unit energy, for neutrons in state $\vec{\mathrm{k}}'$

Using standard "box normalization", the volume per k state is $(2\pi)^3/Y$ where Y = box volume

Final neutron energy is $E'=\frac{\hbar^2k'^2}{2m}\Rightarrow dE'=\frac{\hbar^2k'dk'}{m}$ so

$\rho_{k'}dE'=$ number of wavevector states in volume $k'^2dk'd\Omega=\frac{Y}{(2\pi)^3}k'^2dk'd\Omega$

i.e. $$\rho_{\vec{k}'}=\frac{\text{number of wavevector states}}{\text{dE}'}=\frac{Y}{(2\pi)^3}k'\frac{m}{\hbar^2}d\Omega$$

Further, $\Phi=$ incident flux $=$ density x velocity $=\frac{1}{Y}\frac{\hbar}{m}k$

Fermi pseudopotential

So, $$\frac{d\sigma}{d\Omega}=\frac{Y}{k}\frac{m}{\hbar}\frac{1}{d\Omega}\frac{2\pi}{\hbar}\frac{Y}{(2\pi)^3}k'\frac{m}{\hbar^2}d\Omega\left|\left\langle\vec{k}'\middle|V\middle|\vec{k}\right\rangle\right|^2=\left(\frac{m}{2\pi\hbar^2}\right)^2\left|\int V(\vec{r})e^{i(\vec{k}-\vec{k}').\vec{r}}d\vec{r}\right|^2$$ so $$\boxed{V(\vec{r})=\frac{2\pi\hbar^2}{m}b\delta(\vec{r})}$$

Use V(r) to Calculate the Refractive Index for Neutrons

The nucleus - neutron potential is given by: $V(\vec{r}) = \dfrac{2\pi\hbar^2}{m} b\delta(\vec{r})$ for a single nucleus.

So the average potential inside the medium is: $\bar{V} = \dfrac{2\pi\hbar^2}{m}\rho$ where $\rho = \dfrac{1}{volume}\sum_i b_i$

ρ is called the nuclear Scattering Length Density (SLD) - used for SANS & reflectometry

The kinetic (and total) energy of neutron in vaccuum is $E = \dfrac{\hbar^2 k_0^2}{2m}$

Inside the medium the total energy is $\dfrac{\hbar^2 k^2}{2m} + \bar{V}$

Conservation of energy gives $\dfrac{\hbar^2 k_0^2}{2m} = \dfrac{\hbar^2 k^2}{2m} + \bar{V} = \dfrac{\hbar^2 k^2}{2m} + \dfrac{2\pi\hbar^2}{m}\rho$ or $k_0^2 - k^2 = 4\pi\rho$

Since $k/k_0 = n =$ refractive index (by definition), and ρ is very small ($\sim 10^{-6}$ A^{-2}) we get:

$$\boxed{n = 1 - \lambda^2 \rho / 2\pi}$$

Since generally n < 1, neutrons are externally reflected from most materials.

Why do we Care about the Refractive Index?

- When the wavevector transfer **Q** is small, the phase factors in the cross section do not vary much from nucleus to nucleus & we can use a continuum approximation

- We can use all of the apparatus of optics to calculate effects such as:
  - External reflection from single surfaces (for example from guide surfaces)
  - External reflection from multilayer stacks (including supermirrors)
  - Focusing by (normally) concave lenses or Fresnel lenses
  - The phase change of the neutron wave through a material for applications such as interferometry or phase radiography
  - Fresnel edge enhancement in radiography

Scattering Length Density

- Remember $\frac{d\sigma}{d\Omega} = b_{coh}^2 \left\langle \left| \int d\vec{r}.e^{-i\vec{Q}.\vec{r}} n_{nuc}(\vec{r}) \right|^2 \right\rangle$
- What happens if Q is very small?
  - The phase factor will not change significantly between neighboring atoms
  - We can average the nuclear scattering potential over length scales ~2□/10Q
  - This average is called the scattering length density and denoted $\rho(\vec{r})$
- How do we calculate the SLD?
  - Easiest method: go to www.ncnr.nist.gov/resources/sldcalc.html
  - By hand: let us calculate the scattering length density for quartz – SiO_2
  - Density is 2.66 $gm.cm^{-3}$; Molecular weight is 60.08 gm. $mole^{-1}$
  - Number of molecules per $Å^3$ = N = $10^{-24}(2.66/60.08)*N_{avagadro}$ = 0.0267 molecules per $Å^3$
  - SLD=Σb/volume = $N(b_{Si} + 2b_O) = 0.0267(4.15 + 11.6)\ 10^{-5}\ Å^{-2} = 4.21\ x10^{-6}\ Å^{-2}$
- A uniform SLD causes scattering only at Q=0; variations in the SLD cause scattering at finite values of Q

SLD Calculation

- www.ncnr.nist.gov/resources/sldcalc.html
- Need to know chemical formula and density

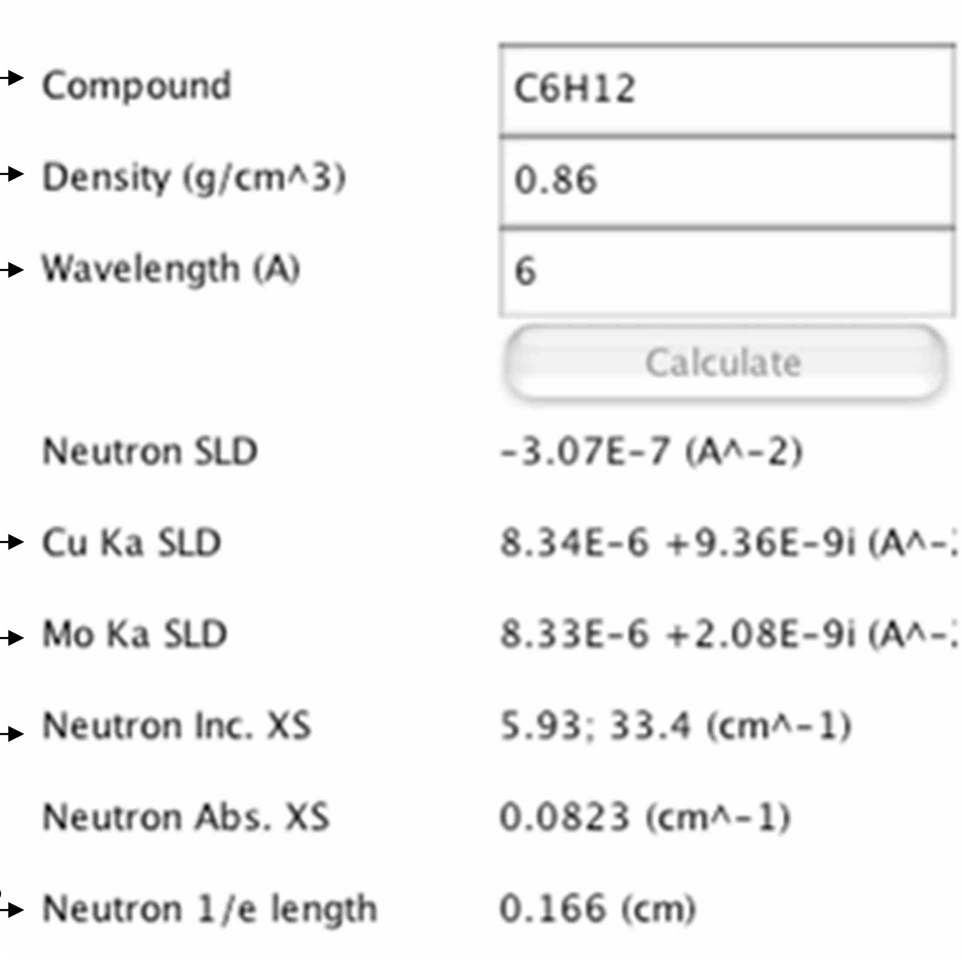
Enter

Not relevant for SLD

X-ray values

Background

Determine best sample thickness



Compound	C6H12
Density (g/cm^3)	0.86
Wavelength (A)	6

Neutron SLD	-3.07E-7 (A^-2)
Cu Ka SLD	8.34E-6 +9.36E-9i (A^-
Mo Ka SLD	8.33E-6 +2.08E-9i (A^-
Neutron Inc. XS	5.93; 33.4 (cm^-1)
Neutron Abs. XS	0.0823 (cm^-1)
Neutron 1/e length	0.166 (cm)

Note units of the cross section – this is cross section per unit volume of sample

Typical SANS/SAXS Applications

- Biology
  - Organization of biomolecular complexes in solution
  - Conformation changes affecting function of proteins, enzymes, protein/DNA complexes, membranes etc
  - Mechanisms and pathways for protein folding and DNA supercoiling

- Polymers
  - Conformation of polymer molecules in solution and in the bulk
  - Structure of microphase separated block copolymers
  - Factors affecting miscibility of polymer blends

- Chemistry
  - Structure and interactions in colloid suspensions, microemeulsions, surfactant phases etc
  - Mechanisms of molecular self-assembly in solutions

Instrumental Resolution for SANS/SAXS

$$Q = \frac{4\pi}{\lambda}\sin\theta \Rightarrow \left\langle \frac{\delta Q}{Q^2}^2 \right\rangle = \left\langle \frac{\delta\lambda^2}{\lambda^2} \right\rangle + \left\langle \frac{\cos^2\theta.\delta\theta^2}{\sin^2\theta} \right\rangle$$

For SANS, $(\delta\lambda/\lambda)_{rms} \sim 5\%$ and θ is small, so $\left\langle \frac{\delta Q}{Q^2}^2 \right\rangle = 0.0025 + \left\langle \frac{\delta\theta^2}{\theta^2} \right\rangle$

For equal source - sample & sample - detector distances of L and equal apertures at source and sample of h, $\delta\theta_{rms} = \sqrt{5/12}\mathrm{h/L}$.

The smallest value of θ is determined by the direct beam size : $2\theta_{\mathrm{min}} \sim 1.5h/L$

At this value of θ, angular resolution dominates and

$\delta \mathrm{Q}_{\mathrm{rms}} \sim (\delta\theta_{\mathrm{rms}}/\theta_{\mathrm{min}})\mathrm{Q}_{\mathrm{min}} \sim \delta\theta_{\mathrm{rms}} 4\pi/\lambda \sim (2\pi/\lambda)h/L$

The largest observable object is $\sim 2\pi/\delta\mathrm{Q}_{\mathrm{rms}} \sim \lambda L/h$.

This achieves a maximum of about 5 μm at the ILL 40 m SANS instrument using 15 Å neutrons.

Note that at the largest values of θ, set by the detector size and distance from the sample, wavelength resolution dominates.

SANS Measures Particle Shapes and Inter-particle Correlations

$$\frac{d\sigma}{d\Omega} = \langle b\rangle^2 \int_{space} d^3r \int_{space} d^3r'\, n_N(\vec{r})\, n_N(\vec{r}\,').e^{i\vec{Q}.(\vec{r}-\vec{r}\,')}$$

$$= \int_{space} d^3R \int_{space} d^3R' \left\langle n_P(\vec{R})\, n_P(\vec{R}') \right\rangle e^{i\vec{Q}.(\vec{R}-\vec{R}')} \left\langle \left| (\rho-\rho_0) \int_{particle} d^3x.e^{i\vec{Q}.\vec{x}} \right|^2 \right\rangle_{orientation}$$

$$\boxed{\frac{d\sigma}{d\Omega} = (\rho-\rho_0)^2 \left|F(\vec{Q})\right|^2 V_p^2 N_P \int_{space} d^3R.G_P(\vec{R}).e^{i\vec{Q}.\vec{R}}}$$

where G_P is the particle - particle correlation function (the probability that there is a particle at $\vec{R}$ if there's one at the origin) and $\left|F(\vec{Q})\right|^2$ is the particle form factor :

$$\boxed{\left|F(\bar{Q})\right|^2 = \frac{1}{V_p^2} \left\langle \left| \int_{particle} d^3x.e^{i\vec{Q}.\vec{x}} \right|^2 \right\rangle_{orientation}}$$

These expressions are the same as those for nuclear scattering except for the addition of a form factor that arises because the scattering is no longer from point-like particles

Scattering from Independent Particles

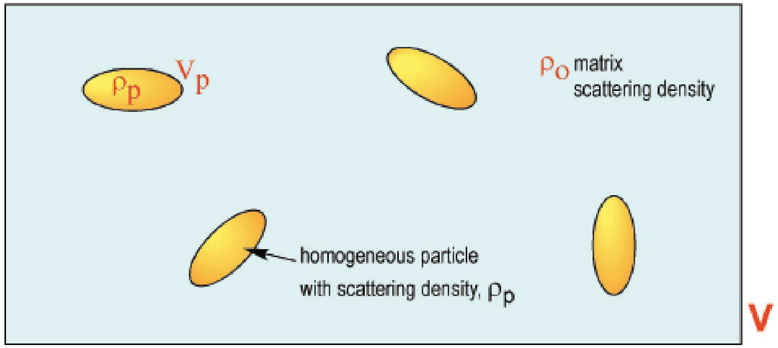
Scattered intensity per unit volume of sample = $I(\vec{Q}) = \frac{1}{V}\frac{d\sigma}{d\Omega} = \frac{1}{V}\left\langle \left| \int \rho(\vec{r}) e^{i\vec{Q}.\vec{r}} d\vec{r} \right|^2 \right\rangle$

For identical particles

$$I(Q) = \frac{N}{V}(\rho_p - \rho_0)^2 V_p^2 \left\langle \left| \frac{1}{V_p} \int_{particle} e^{i\vec{Q}.\vec{r}} d\vec{r} \right|^2 \right\rangle$$

contrast factor

particle form factor $|F(\vec{Q})|^2$



Note that $I(0) = \frac{N}{V}(\rho_p - \rho_0)^2 V_p^2$

Particle concentration $c = NV_p / V$ and particle molecular weight $M_w = \rho V_p N_A$

where ρ is the particle mass density and N_A is Avagadro's number

so $I(0) = \frac{cM_w}{\rho N_A}(\rho_p - \rho_0)^2$ provides a way to find the particle molecular weight

Scattering for Spherical Particles

The particle form factor $\left|F(\vec{Q})\right|^2 = \left|\int_V d\vec{r}\, e^{i\vec{Q}.\vec{r}}\right|^2$ is determined by the particle shape.

For a sphere of radius R, F(Q) only depends on the magnitude of Q:

$$\boxed{F_{sphere}(Q) = 3V_0\left[\frac{\sin QR - QR\cos QR}{(QR)^3}\right] \equiv \frac{3V_0}{QR}\, j_1(QR) \rightarrow V_0 \text{ at } Q = 0}$$

Thus, as Q → 0, the total scattering from an assembly of uncorrelated spherical particles [i.e. when $G(\vec{r}) \rightarrow \delta(\vec{r})$] is proportional to the square of the particle volume times the number of particles.

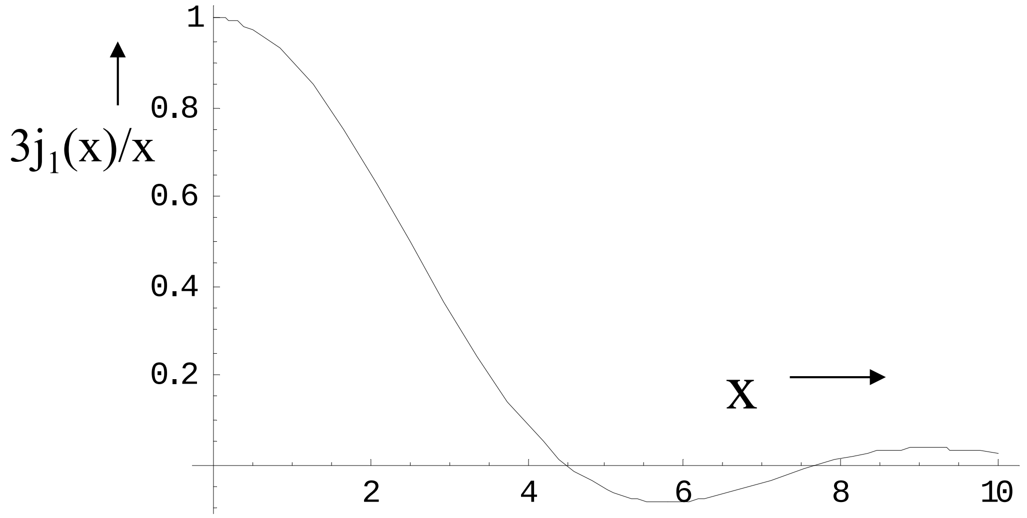
For elliptical particles

replace R by:

$R \rightarrow (a^2 \sin^2\vartheta + b^2 \cos^2\vartheta)^{1/2}$

where ϑ is the angle between

the major axis (a) and $\vec{Q}$



Radius of Gyration Is the Particle “Size” Usually Deduced From SANS Measurements

If we measure $\vec{r}$ from the centroid of the particle and expand the exponential in the definition of the form factor at small Q :

$$F(Q)=\int_V d\vec{r}e^{i\vec{Q}.\vec{r}} \approx V_0 + \cancel{i\int_V \vec{Q}.\vec{r}d^3r} - \frac{1}{2}\int_V (\vec{Q}.\vec{r})^2 d^3r + ...$$

$$= V_0\left[1-\frac{Q^2}{2}\frac{\int_0^\pi \cos^2\theta\sin\theta.d\theta}{\int_0^\pi \sin\theta.d\theta}\frac{\int_{V_0} r^2d^3r}{\int_{V_0}d^3r}+...\right] = V_0\left[1-\frac{Q^2r_g^2}{6}+...\right]\approx V_0e^{-\frac{Q^2r_g^2}{6}}$$

where r_g is the radius of gyration is $r_g = \int_V R^2d^3r / \int_V d^3r$. It is usually obtained from a fit to SANS data at low Q (in the so-called Guinier region) or by plotting ln(Intensity) v Q^2. The slope of the data at the lowest values of Q is $r_g^2/3$. It is easily verified that the expression for the form factor of a sphere is a special case of this general result.

Shape Determination for Dilute, Randomly Oriented, Uniform Particles

$$I(Q) = \frac{N}{V}(\rho_p - \rho_0)^2 \left\langle \left| \int_{V_p} e^{i\vec{Q}.\vec{r}}\, d\vec{r} \right|^2 \right\rangle = \frac{N}{V}(\rho_p - \rho_0)^2 \left\langle \int_{V_p} e^{i\vec{Q}.\vec{r}}\, d\vec{r} \int_{V_p} e^{-i\vec{Q}.\vec{r}'}\, d\vec{r}' \right\rangle$$

$$I(Q) = \frac{N}{V}(\rho_p - \rho_0)^2 \left\langle \int_{V_p} e^{i\vec{Q}.(\vec{r}-\vec{r}')}\, d(\vec{r}-\vec{r}') V_p \right\rangle = (\rho_p - \rho_0)^2 \left\langle \int_{V_p} \gamma(\vec{R}) e^{i\vec{Q}.\vec{R}}\, d\vec{R} \right\rangle_{orientation}$$

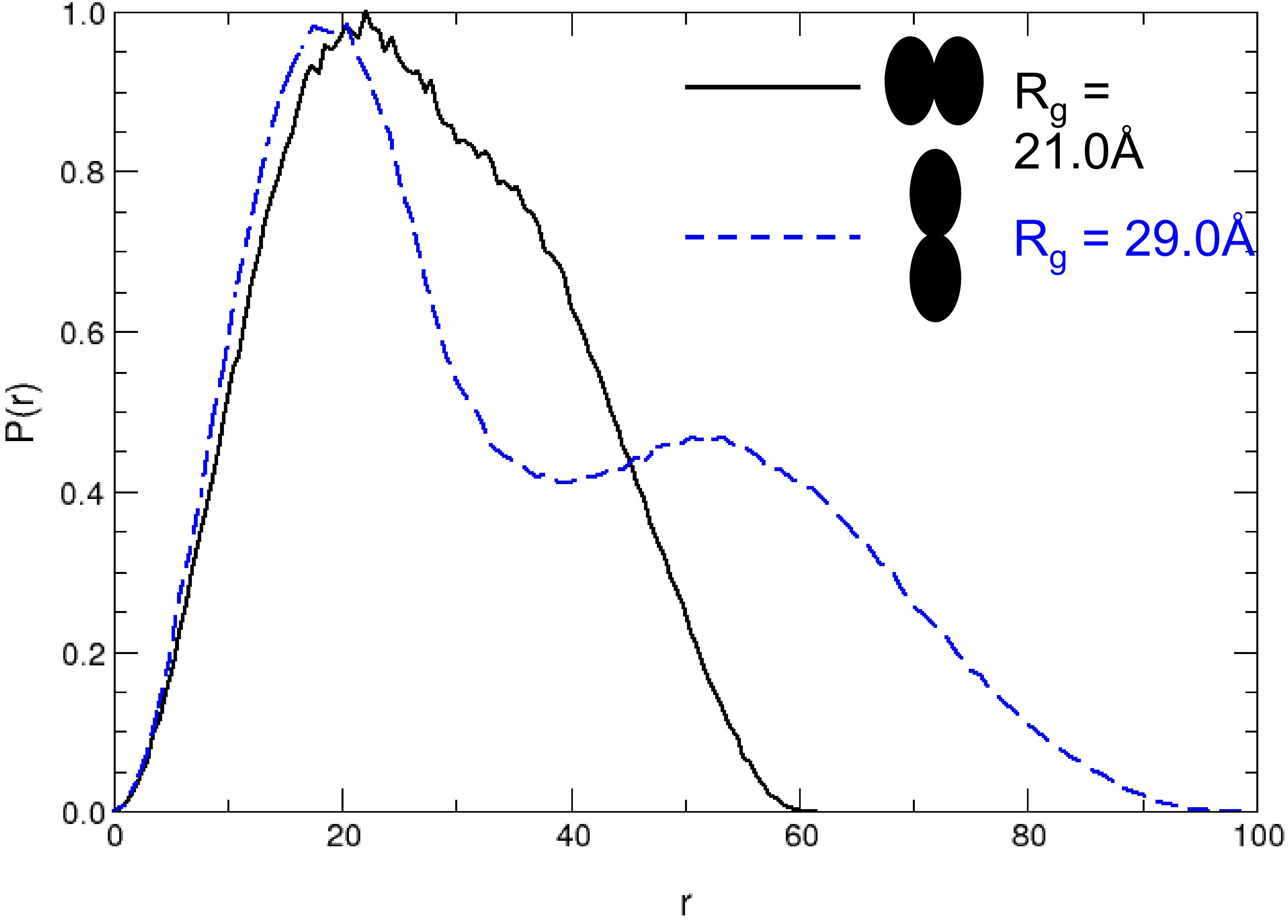
$$I(Q) = (\rho_p - \rho_0)^2 4\pi \int_0^{D_{\max}} r^2 \gamma(r) \frac{\sin Qr}{Qr}\, dr$$

where $\mathrm{P(r)} \equiv 4\pi\mathrm{r}^2\gamma(\mathrm{r})$ is the probability of finding two points in the particle separated by r

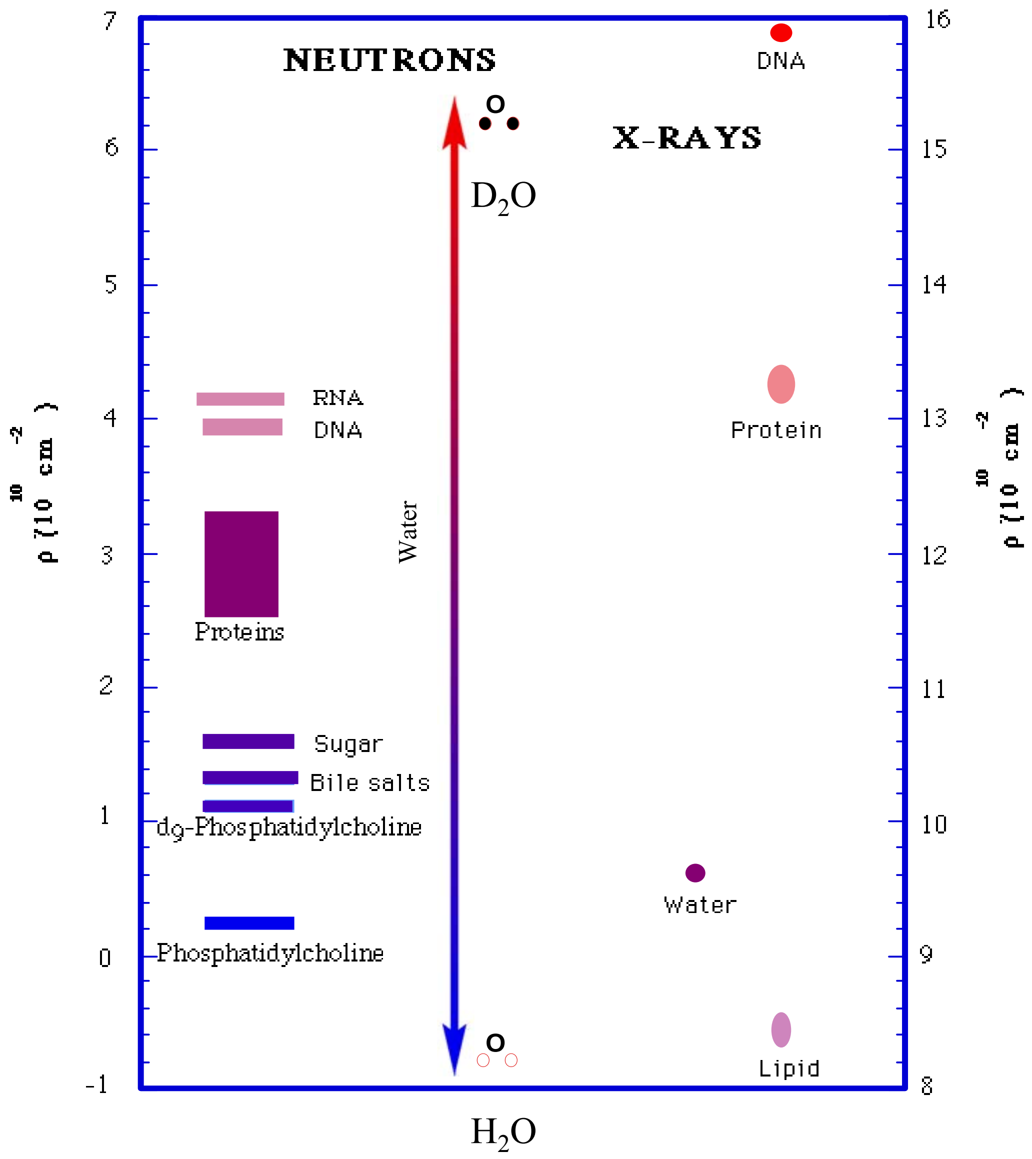
- If I(Q) is measured over a wide enough Q range then the inverse transform can be computed

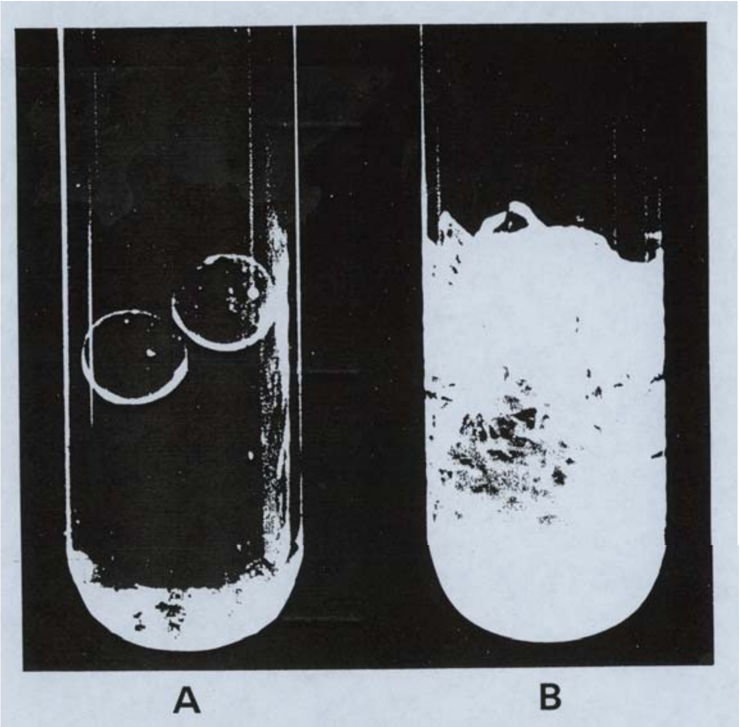
$$P(r) \equiv 4\pi r^2 \gamma(r) = \frac{2}{\pi} \int QI(Q) \sin(Qr)\, dQ$$

P(r) for Simple Models



Contrast & Contrast Matching

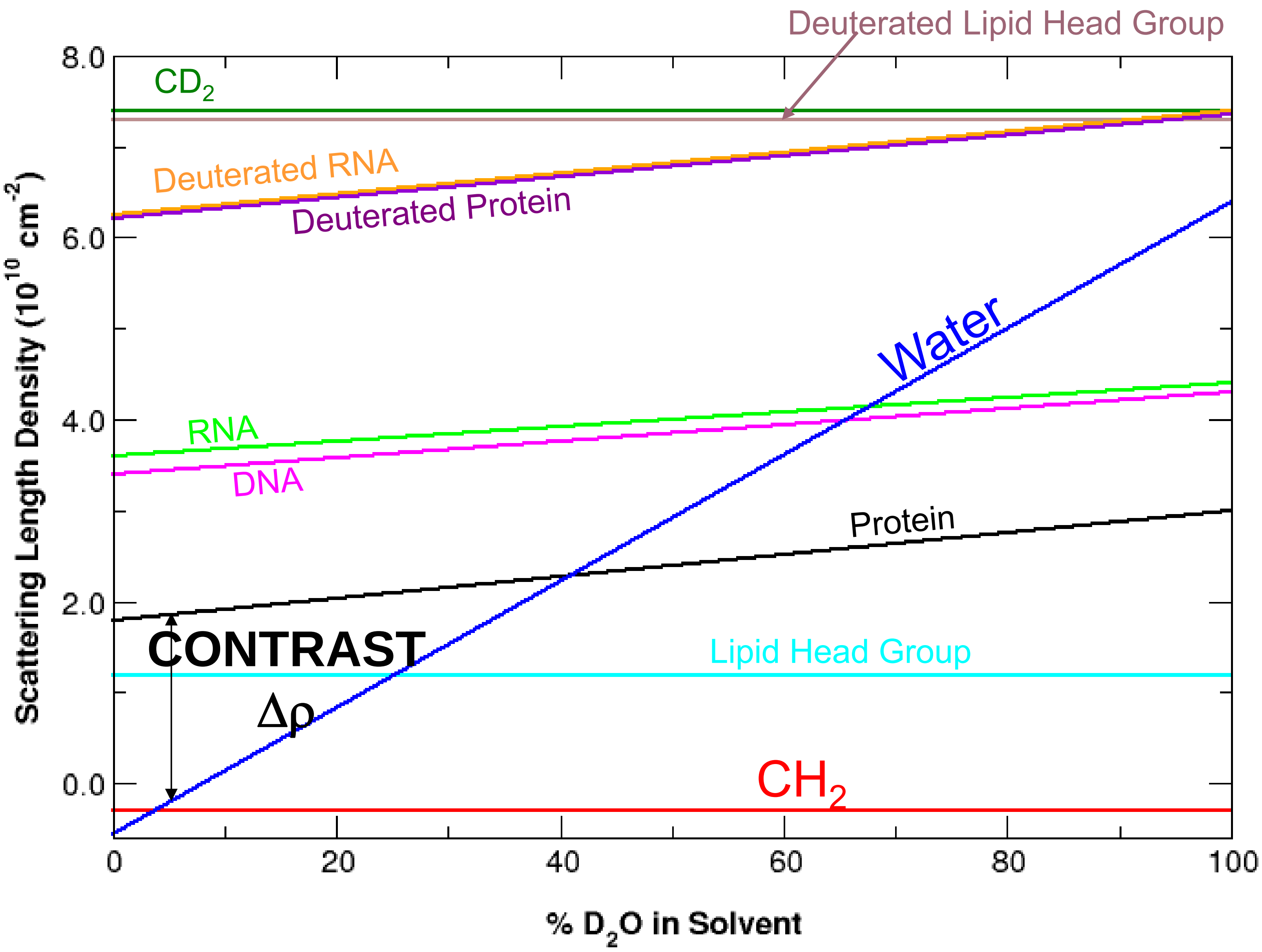




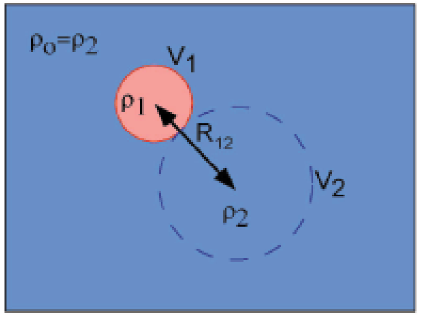
Both tubes contain borosilicate beads + pyrex fibers + solvent. (A) solvent refractive index matched to pyrex;. (B) solvent index different from both beads and fibers – scattering from fibers dominates

* Chart courtesy of Rex Hjelm

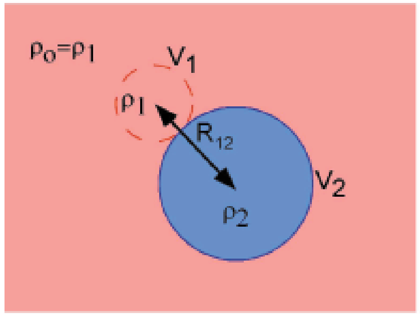
Contrast Variation



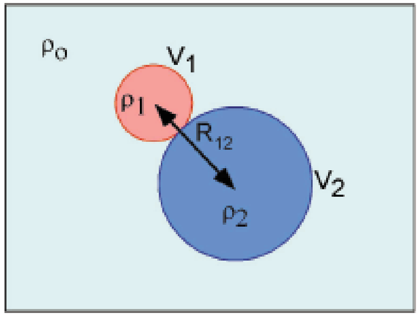
Using Contrast Variation to Study Compound Particles



$$I_1(Q) = (\rho_1 - \rho_2)^2 F_1^2$$



$$I_2(Q) = (\rho_2 - \rho_1)^2 F_2^2$$



$$I_3(Q) - \frac{(\rho_1 - \rho_o)^2}{(\rho_1 - \rho_2)^2} I_1(Q) - \frac{(\rho_2 - \rho_o)^2}{(\rho_1 - \rho_2)^2} I_2(Q)$$

$$= \underbrace{2(\rho_1 - \rho_o)(\rho_2 - \rho_o) F_1 F_2 \frac{\sin(QR_{12})}{QR_{12}}}_{=0 \text{ at } Q = \pi/R_{12}}$$

Examples include nucleosomes (protein/DNA) and ribosomes (poteins/RNA)

$$I(Q) = \frac{N}{V}\left\langle \left| \Delta\rho_1 \int_{V_1} e^{i\vec{Q}.\vec{r}} d\vec{r}_1 + \Delta\rho_2 \int_{V_2} e^{i\vec{Q}.\vec{r}} d\vec{r}_2 \right|^2 \right\rangle$$

$$I(Q) = \Delta\rho_1^2 \left\langle |F_1(Q)|^2 \right\rangle + \Delta\rho_2^2 \left\langle |F_2(Q)|^2 \right\rangle +$$

$$\Delta\rho_1 \Delta\rho_2 |F_1(Q)||F_2(Q)| \frac{\sin(QR_{12})}{QR_{12}}$$

Viewgraph from Charles Glinka (NIST)

Porod Scattering

Let us examine the behavior of $|\mathrm{F(Q)}|^2 (QR)^4$ at large values of Q for a spherical particle (i.e. $\mathrm{Q} >> 1/\mathrm{R}$ where R is the sphere radius)

$$|F(Q)|^2 (QR)^4 = 9V^2 \left[\frac{\sin QR - QR.\cos QR}{(QR)^3} \right]^2 (QR)^4 = 9V^2 \left[\frac{\sin QR}{QR} - \cos QR \right]^2$$

$$\rightarrow 9V^2 \cos^2 QR \text{ as } \mathrm{Q} \rightarrow \infty$$

$$= 9V^2/2 \text{ on average (the oscillations will be smeared out by resolution)}$$

Thus $\boxed{|F(Q)|^2 \rightarrow \frac{9V^2}{2(QR)^4} = \frac{2\pi A}{Q^4}}$ where A is the area of the sphere's surface.

This is Porod's law and holds as $\mathrm{Q} \rightarrow \infty$ for any particle shape provided the particle surface is smooth.

Another way to obtain it is to expand $\mathrm{G(r) = 1 - ar + br^2 + ..}$[with $\mathrm{a = A/(2\pi V)}$] at small r and to evaluate the form factor with this (Debye) form for the correlation function.

Scattering From Fractal Systems

- Fractals are systems that are “self-similar” under a change of scale I.e. R -> CR
- For a mass fractal the number of particles within a sphere of radius R is proportional to R^D where D is the fractal dimension

Thus

$$4\pi R^2 dR.G(R) = \text{number of particles between distance R and R + dR} = cR^{D-1}dR$$

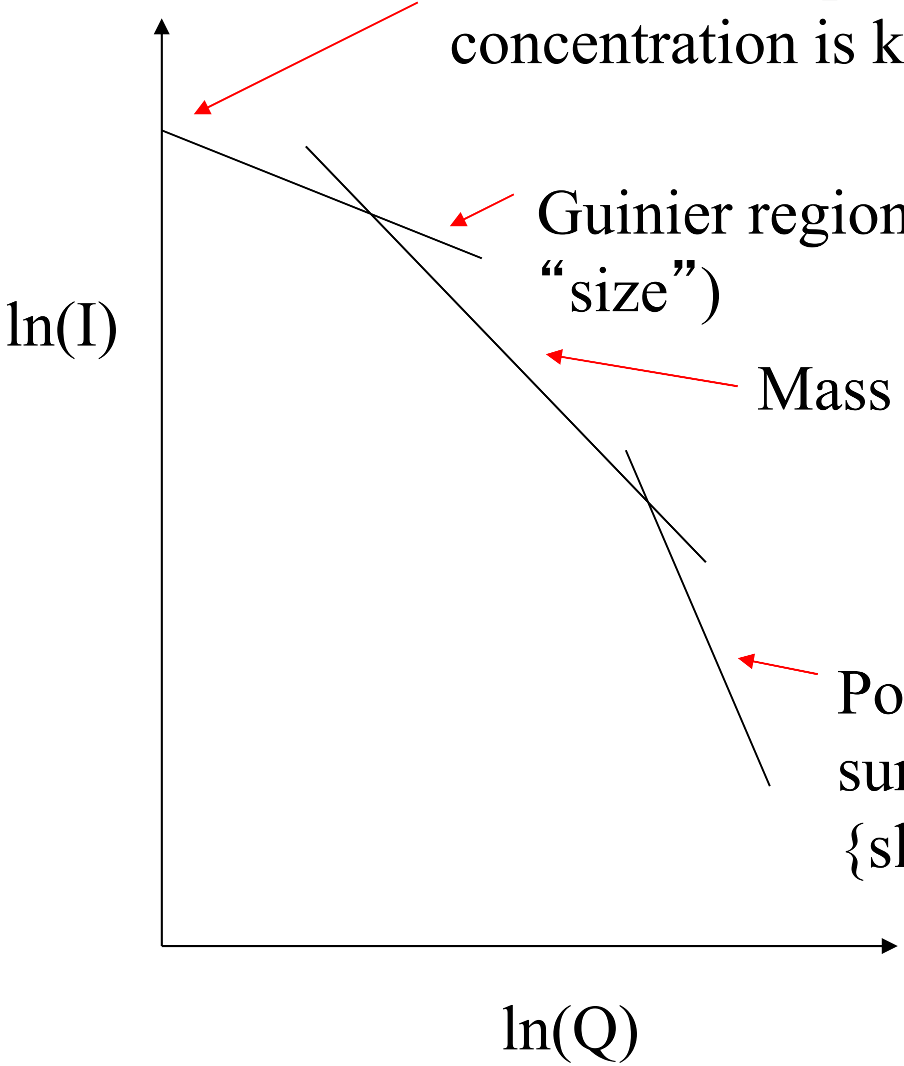
$$\therefore \; G(R) = (c/4\pi)R^{D-3}$$

$$\text{and} \;\; S(\vec{Q}) = \int d\vec{R}.e^{i\vec{Q}.\vec{R}}G(R) = \frac{2\pi}{Q}\int dR.R.\sin QR.(c/4\pi)R^{D-3}$$

$$= \frac{c}{2}\frac{1}{Q^D}\int dx.x^{D-2}.\sin x = \frac{const}{Q^D}$$

For a surface fractal, one can prove that $S(Q) \propto \dfrac{const}{Q^{6-D_s}}$ which reduces to the Porod form for smooth surfaces of dimension 2.

Typical Intensity Plot for SANS From Disordered Systems



Zero Q intercept - gives particle volume if concentration is known

Guinier region (slope = $-r_g^2/3$ gives particle “size”)

Mass fractal dimension (slope = -D)

Porod region - gives surface area and surface fractal dimension {slope = $-(6-D_s)$}

General References

- Introduction to the Theory of Thermal Neutron Scattering
  by G. L. Squires
- Neutron Scattering: A Non-Destructive Microscope for Seeing Inside Matter
  by Roger Pynn
  Available on-line at http://www.springerlink.com/content/978-0-387-09415-1
- Elements of Modern X-Ray Physics
  by Jens Als-Nielsen and Des McMorrow
  John Wiley and Sons: ISBN 0471498580
- Elementary Scattering Theory For X-ray and Neutron Users
  by D.S. Sivia
  Oxford University Press
- International Neutron Scattering Instrumentation School (INSIS)
  http://neutrons.ornl.gov/conf/insis2012/

SANS References

- A website of SANS tutorials
    - www.ncnr.nist.gov/programs/sans/tutorials

- SANS data can be simulated for various particle shapes using the programs available at:
    - www.ncnr.nist.gov/resources/simulator.html

- To choose instrument parameters for a SANS experiment at NIST go to:
    - www.ncnr.nist.gov/resources/sansplan.html

END

Derivation

The $\vec{\mathrm{B}}$ field at distance $\vec{\mathrm{R}}$ from a magnetic moment $\vec{\mathrm{M}}$ is $\frac{\mu_0}{4\pi}\vec{\nabla}\Lambda\left(\frac{\vec{M}\Lambda\vec{R}}{R^3}\right) = -\frac{\mu_0}{4\pi}\vec{\nabla}\Lambda\left(\vec{M}\Lambda\nabla(1/R)\right)$

Since $\int\frac{1}{q^2}\exp(i\vec{q}.\vec{R})d\vec{q} = 2\pi\int_0^\infty dq\int_{-1}^{1}\exp(iqR\cos\theta)d(\cos\theta) = 4\pi\int_0^\infty\frac{\sin(qR)}{qR}dq = \frac{2\pi^2}{R}$

$$\vec{\nabla}\Lambda\left(\frac{\vec{M}\Lambda\vec{R}}{R^3}\right) = -\frac{1}{2\pi^2}\int\frac{1}{q^2}\vec{\nabla}\Lambda\left(\vec{M}\Lambda\nabla\{\exp i\vec{q}.\vec{R}\}\right)d\vec{q}$$

But $\vec{M}\Lambda\nabla\{\exp i\vec{q}.\vec{R}\} = i\vec{M}\Lambda\vec{q}\exp i\vec{q}.\vec{R}$ and $\vec{\nabla}\Lambda\vec{M}\Lambda\vec{q}\exp i\vec{q}.\vec{R} = i\vec{q}\Lambda\vec{M}\Lambda\vec{q}\exp i\vec{q}.\vec{R}$

so $\vec{\nabla}\Lambda\left(\frac{\vec{M}\Lambda\vec{R}}{R^3}\right) = \frac{1}{2\pi^2}\int\frac{1}{q^2}\vec{q}\Lambda\left(\vec{M}\Lambda\vec{q}\right)\{\exp i\vec{q}.\vec{R}\}d\vec{q} = \frac{1}{2\pi^2}\int\vec{M}_\perp(\vec{q})\{\exp i\vec{q}.\vec{R}\}d\vec{q}$

Neutron Scattering Instrumentation is Designed to Compromise between Intensity & Resolution

- Maxwellian distribution of neutron velocities $P(v) \sim \frac{1}{T^{3/2}} e^{-\frac{1}{2}mv^2/kT}$
- Liouville's theorem – the (6-dimensional) phase space density of non-interacting particles cannot be increased by conservative forces
  - Brighter sources => colder moderators or non-equilibrium neutron production
- We can only increase scattered intensity at a given ($\vec{Q}$,E) by increasing the phase space volume
- Design instruments to have good resolution in the direction of ($\vec{Q}$,E) space that is important for the science
- Neutron optics & instrumentation is designed to:
  - Maintain neutron brightness
  - Provide good resolution in a chosen direction in ($\vec{Q}$,E) space
  - Simultaneously measure as many resolution elements [i.e. ($\vec{Q}$,E) points] as is useful

The Intermediate Scattering Function

- Another function that is often useful is the Intermediate Scattering Function defined as

  $$\boxed{I(\vec{Q},t) = \int G(\vec{r},t) e^{i\vec{Q}.\vec{r}} d\vec{r}}$$

  This is the quantity measured with Neutron Spin Echo (NSE)

- It is not possible to derive exact expressions for I, G or S except for simple models. It is therefore useful to know the various analytical properties of these functions to ensure that models preserve them. Squires shows:

  $$I(\vec{Q},t) = I^*(\vec{Q},-t); \qquad I(\vec{Q},t) = I(-\vec{Q},-t+i\hbar/k_BT)$$

  $$G(\vec{r},t) = G^*(-\vec{r},-t); \qquad G(\vec{r},t) = G(-\vec{r},-t+i\hbar/k_BT)$$

  $$S(\vec{Q},\omega) = S^*(\vec{Q},\omega); \qquad S(\vec{Q},\omega) = e^{\hbar\omega/k_BT} S(-\vec{Q},-\omega)$$

- There are also various sum & moment rules on these quantities that are sometimes useful (see Squires for details)