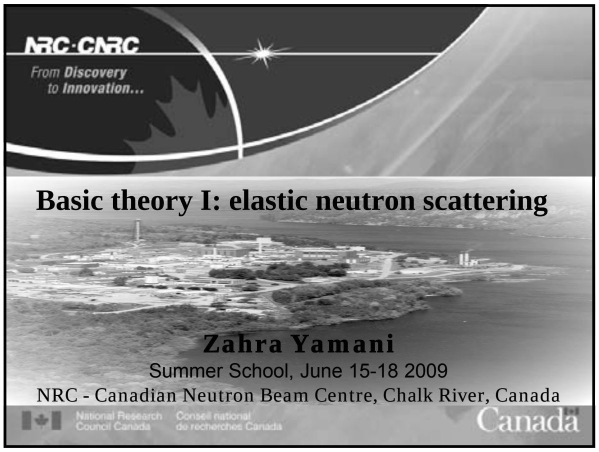


NRC·CNRC

From Discovery to Innovation...

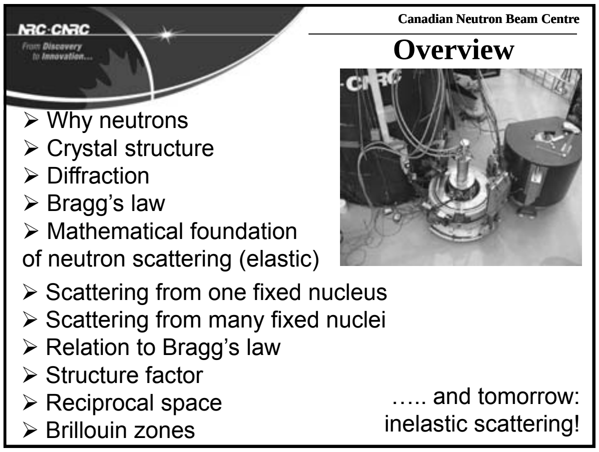
Basic theory I: elastic neutron scattering

Zahra Yamani

Summer School, June 15-18 2009

NRC - Canadian Neutron Beam Centre, Chalk River, Canada

National Research Council Canada · Conseil national de recherches Canada · Canada

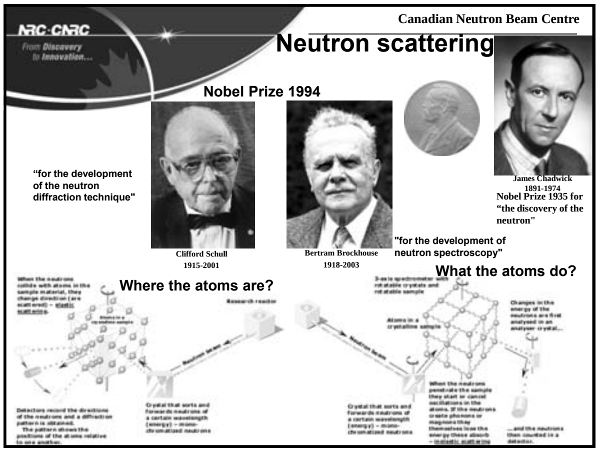


Canadian Neutron Beam Centre

Overview

- Why neutrons
- Crystal structure
- Diffraction
- Bragg's law
- Mathematical foundation of neutron scattering (elastic)
- Scattering from one fixed nucleus
- Scattering from many fixed nuclei
- Relation to Bragg's law
- Structure factor
- Reciprocal space
- Brillouin zones

….. and tomorrow: inelastic scattering!



Canadian Neutron Beam Centre

Neutron scattering

Nobel Prize 1994

"for the development of the neutron diffraction technique"

Clifford Schull
1915-2001

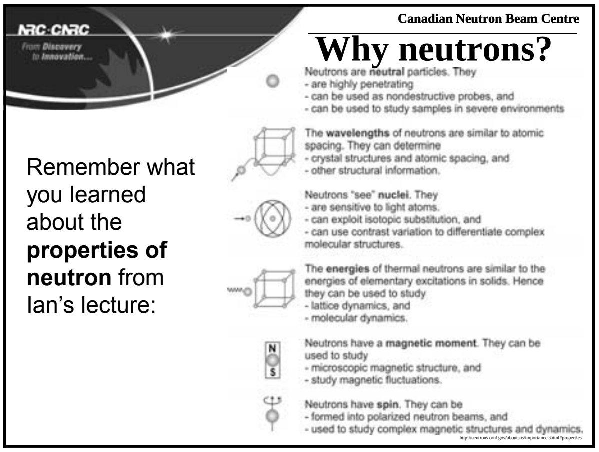
Bertram Brockhouse
1918-2003

"for the development of neutron spectroscopy"

James Chadwick
1891-1974
Nobel Prize 1935 for "the discovery of the neutron"

Where the atoms are?

What the atoms do?



Canadian Neutron Beam Centre

Why neutrons?

Remember what you learned about the **properties of neutron** from Ian's lecture:

Neutrons are **neutral** particles. They
- are highly penetrating
- can be used as nondestructive probes, and
- can be used to study samples in severe environments

The **wavelengths** of neutrons are similar to atomic spacing. They can determine
- crystal structures and atomic spacing, and
- other structural information.

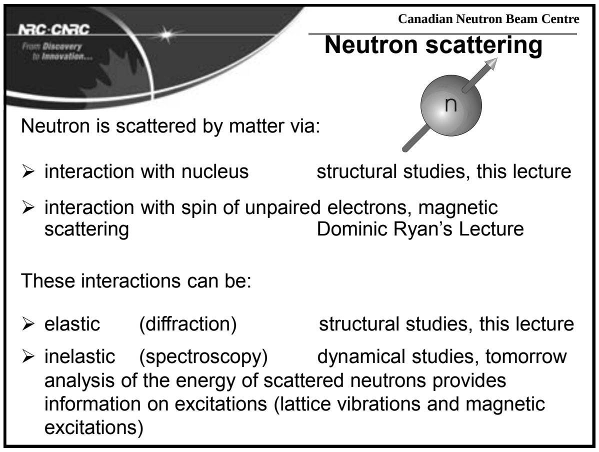
Neutrons "see" **nuclei**. They
- are sensitive to light atoms.
- can exploit isotopic substitution, and
- can use contrast variation to differentiate complex molecular structures.

The **energies** of thermal neutrons are similar to the energies of elementary excitations in solids. Hence they can be used to study
- lattice dynamics, and
- molecular dynamics.

Neutrons have a **magnetic moment**. They can be used to study
- microscopic magnetic structure, and
- study magnetic fluctuations.

Neutrons have **spin**. They can be
- formed into polarized neutron beams, and
- used to study complex magnetic structures and dynamics.

http://neutrons.ornl.gov/aboutsns/importance.shtml#properties



Canadian Neutron Beam Centre

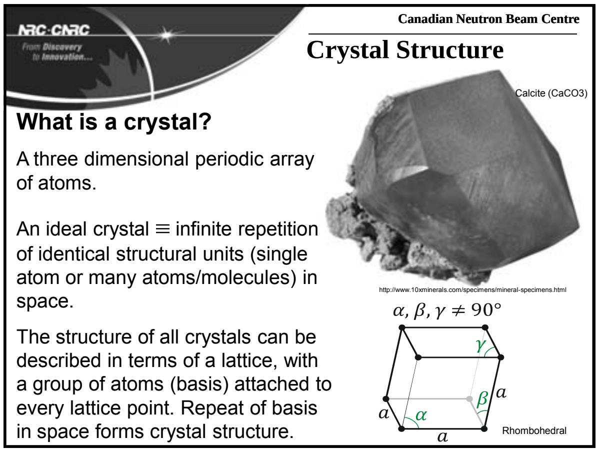
Neutron scattering

Neutron is scattered by matter via:

- interaction with nucleus structural studies, this lecture
- interaction with spin of unpaired electrons, magnetic scattering Dominic Ryan's Lecture

These interactions can be:

- elastic (diffraction) structural studies, this lecture
- inelastic (spectroscopy) dynamical studies, tomorrow analysis of the energy of scattered neutrons provides information on excitations (lattice vibrations and magnetic excitations)



Canadian Neutron Beam Centre

Crystal Structure

Calcite (CaCO3)

What is a crystal?

A three dimensional periodic array of atoms.

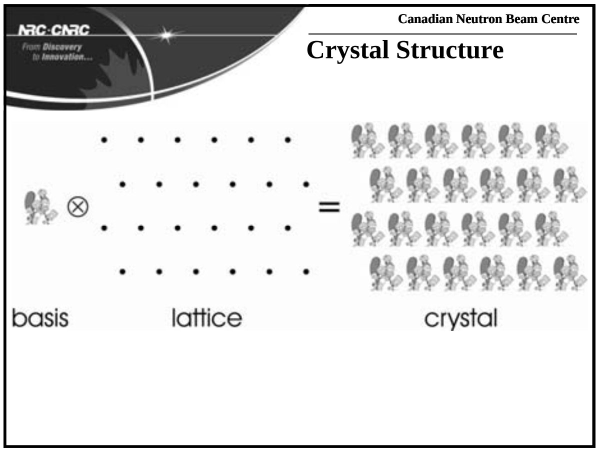
An ideal crystal ≡ infinite repetition of identical structural units (single atom or many atoms/molecules) in space.

The structure of all crystals can be described in terms of a lattice, with a group of atoms (basis) attached to every lattice point. Repeat of basis in space forms crystal structure.

http://www.10xminerals.com/specimens/mineral-specimens.html

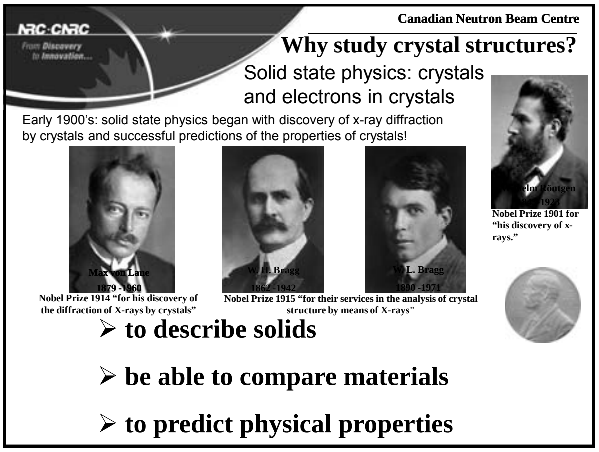
$\alpha, \beta, \gamma \neq 90°$

Rhombohedral



Canadian Neutron Beam Centre

Crystal Structure



Canadian Neutron Beam Centre

Why study crystal structures?

Solid state physics: crystals and electrons in crystals

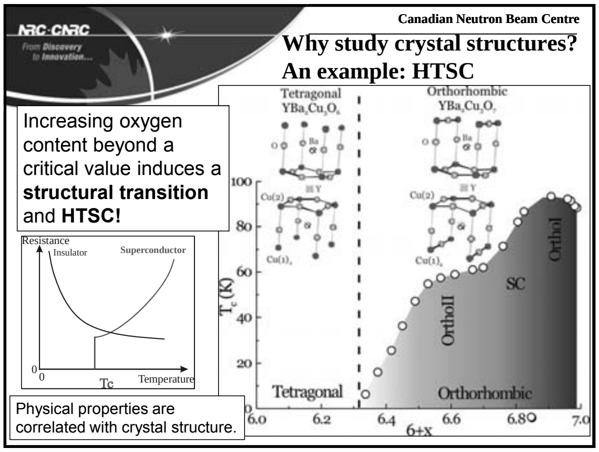
Early 1900's: solid state physics began with discovery of x-ray diffraction by crystals and successful predictions of the properties of crystals!

Nobel Prize 1914 "for his discovery of the diffraction of X-rays by crystals"

Nobel Prize 1915 "for their services in the analysis of crystal structure by means of X-rays"

Nobel Prize 1901 for "his discovery of x-rays."

- ➢ **to describe solids**
- ➢ **be able to compare materials**
- ➢ **to predict physical properties**

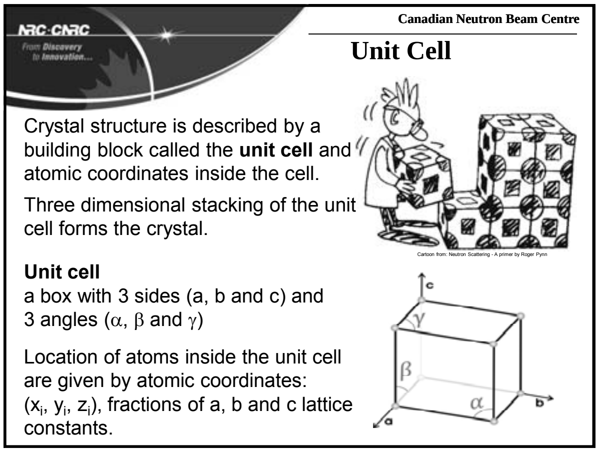


Canadian Neutron Beam Centre

Why study crystal structures? An example: HTSC

Increasing oxygen content beyond a critical value induces a **structural transition** and **HTSC!**

Physical properties are correlated with crystal structure.



Canadian Neutron Beam Centre

Unit Cell

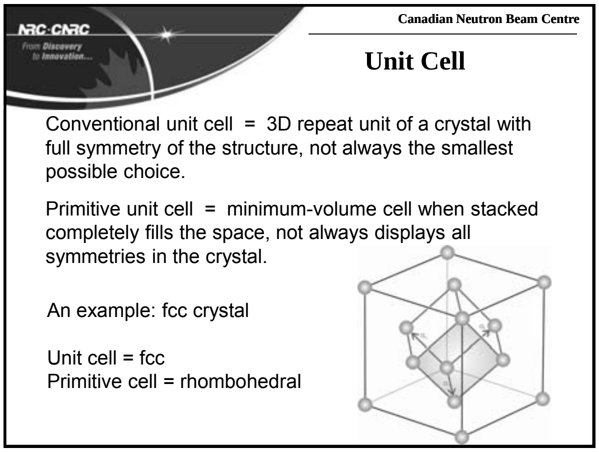
Crystal structure is described by a building block called the **unit cell** and atomic coordinates inside the cell.

Three dimensional stacking of the unit cell forms the crystal.

Cartoon from: Neutron Scattering - A primer by Roger Pynn

Unit cell
a box with 3 sides (a, b and c) and
3 angles (α, β and γ)

Location of atoms inside the unit cell are given by atomic coordinates: (x_i, y_i, z_i), fractions of a, b and c lattice constants.



Canadian Neutron Beam Centre

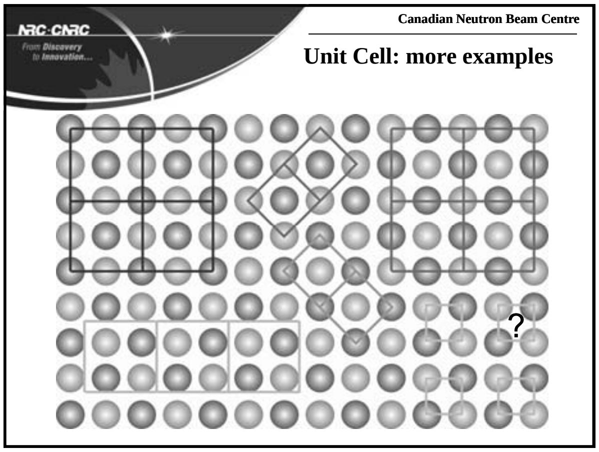
Unit Cell

Conventional unit cell = 3D repeat unit of a crystal with full symmetry of the structure, not always the smallest possible choice.

Primitive unit cell = minimum-volume cell when stacked completely fills the space, not always displays all symmetries in the crystal.

An example: fcc crystal

Unit cell = fcc
Primitive cell = rhombohedral



Canadian Neutron Beam Centre

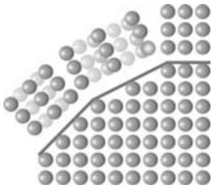
Unit Cell: more examples

Lattice planes & Miller indices

Periodic arrangement forms planes of atoms.

Crystallographic directions = imaginary lines connecting atoms. Crystallographic planes = imaginary planes connecting atoms in different directions.

Some directions and planes have a higher density of atoms.

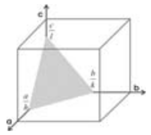


d-spacing = perpendicular distance between pairs of nearest planes.

All planes in one direction are identical.

How to identify/label the planes:
Miller indices

Lattice planes & Miller indices



Miller indices (***h k l***) = three lattice points used to identify orientation of a set of parallel planes of atoms within a crystal structure.

(h k l) plane intercepts crystallographic axes **a**, **b** and **c** at

$\frac{a}{h}, \frac{b}{k}, \frac{c}{l}$ intercepts → what an index=0 means?

where *h*, *k*, and *l* are relatively prime integers

$\frac{1}{h}, \frac{1}{k}, \frac{1}{l}$ fractional intercepts

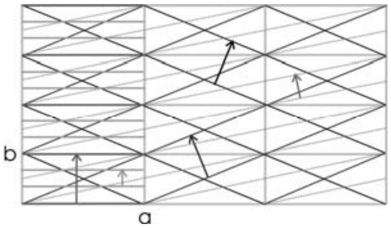
We will come back to this

h, k, l reciprocals of fractional intercepts

Miller indices

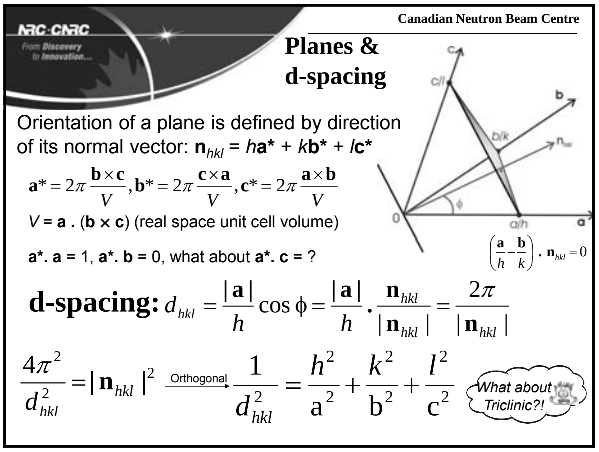
Lattice planes & Miller indices examples:

Planes separated by one unit cell or a fraction of a unit cell pass through equivalent atoms throughout the crystal.



Can you identify (010), (030), (110), (-110) and (120) planes?

Notice larger Miller indices mean closer spacings (**reciprocal**)!



Planes & d-spacing

Orientation of a plane is defined by direction of its normal vector: $\mathbf{n}_{hkl} = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^*$

$$\mathbf{a}^* = 2\pi\frac{\mathbf{b}\times\mathbf{c}}{V}, \mathbf{b}^* = 2\pi\frac{\mathbf{c}\times\mathbf{a}}{V}, \mathbf{c}^* = 2\pi\frac{\mathbf{a}\times\mathbf{b}}{V}$$

$V = \mathbf{a}\ .\ (\mathbf{b}\times\mathbf{c})$ (real space unit cell volume)

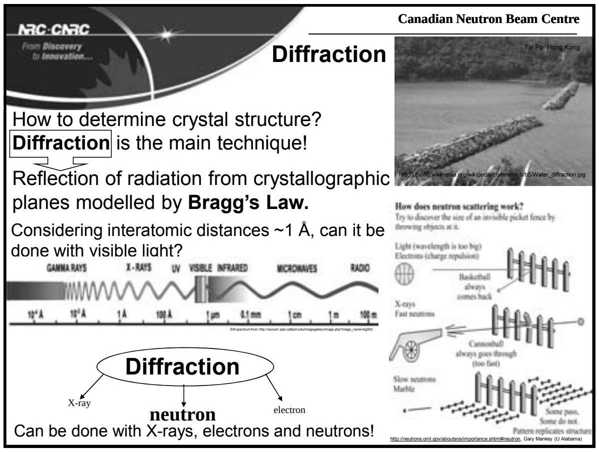
$\mathbf{a}^*.\ \mathbf{a} = 1$, $\mathbf{a}^*.\ \mathbf{b} = 0$, what about $\mathbf{a}^*.\ \mathbf{c} = ?$

$$\left(\frac{\mathbf{a}}{h}-\frac{\mathbf{b}}{k}\right) .\ \mathbf{n}_{hkl} = 0$$

d-spacing: $d_{hkl} = \frac{|\mathbf{a}|}{h}\cos\phi = \frac{|\mathbf{a}|}{h} . \frac{\mathbf{n}_{hkl}}{|\mathbf{n}_{hkl}|} = \frac{2\pi}{|\mathbf{n}_{hkl}|}$

$$\frac{4\pi^2}{d_{hkl}^2} = |\mathbf{n}_{hkl}|^2 \xrightarrow{\text{Orthogonal}} \frac{1}{d_{hkl}^2} = \frac{h^2}{\mathrm{a}^2} + \frac{k^2}{\mathrm{b}^2} + \frac{l^2}{\mathrm{c}^2}$$

What about Triclinic?!



Diffraction

How to determine crystal structure?

Diffraction is the main technique!

Reflection of radiation from crystallographic planes modelled by **Bragg's Law.**

Considering interatomic distances ~1 Å, can it be done with visible light?

EM spectrum from: http://sscws1.ipac.caltech.edu/imagegallery/image.php?image_name=bg002

Diffraction

X-ray

neutron

electron

Can be done with X-rays, electrons and neutrons!

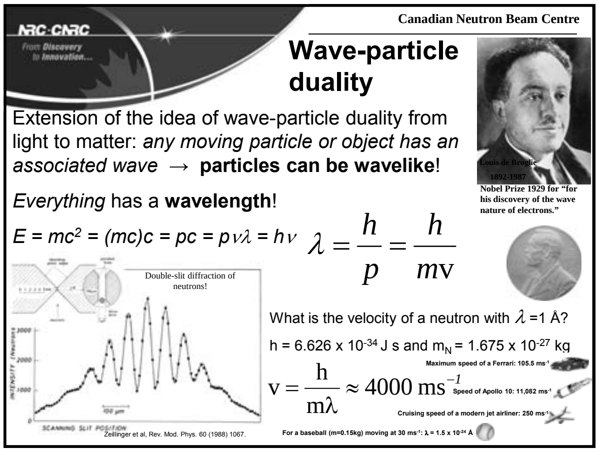
Tai Po, Hong Kong

http://upload.wikimedia.org/wikipedia/commons/b/b5/Water_diffraction.jpg

How does neutron scattering work?

Try to discover the size of an invisible picket fence by throwing objects at it.

http://neutrons.ornl.gov/aboutsns/importance.shtml#neutron, Gary Mankey (U Alabama)



Wave-particle duality

Extension of the idea of wave-particle duality from light to matter: *any moving particle or object has an associated wave* → **particles can be wavelike**!

Everything has a **wavelength**!

$E = mc^2 = (mc)c = pc = p\nu\lambda = h\nu$

$$\lambda = \frac{h}{p} = \frac{h}{m\mathrm{v}}$$

Louis de Broglie
1892-1987

Nobel Prize 1929 for "for his discovery of the wave nature of electrons."

Double-slit diffraction of neutrons!

Zeillinger et al, Rev. Mod. Phys. 60 (1988) 1067.

What is the velocity of a neutron with λ =1 Å?

h = 6.626 x 10^{-34} J s and m_N = 1.675 x 10^{-27} kg

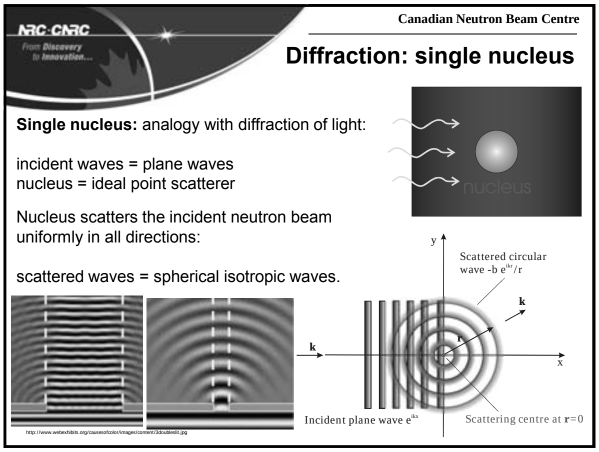
$$\mathrm{v} = \frac{\mathrm{h}}{\mathrm{m}\lambda} \approx 4000\ \mathrm{ms}^{-1}$$

Maximum speed of a Ferrari: 105.5 ms^{-1}

Speed of Apollo 10: 11,082 ms^{-1}

Cruising speed of a modern jet airliner: 250 ms^{-1}

For a baseball (m=0.15kg) moving at 30 ms^{-1}: λ = 1.5 x 10^{-24} Å



Canadian Neutron Beam Centre

Diffraction: single nucleus

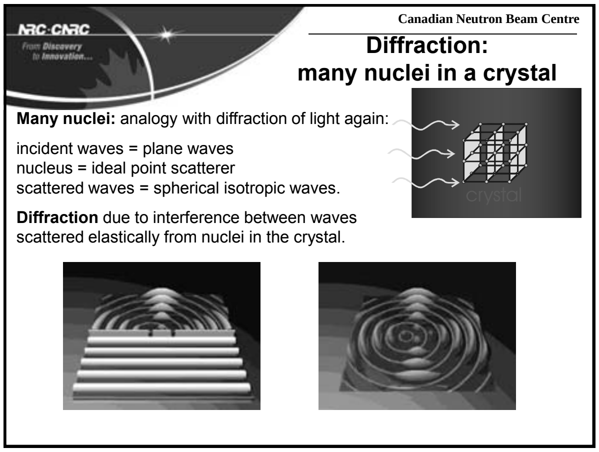
Single nucleus: analogy with diffraction of light:

incident waves = plane waves
nucleus = ideal point scatterer

Nucleus scatters the incident neutron beam uniformly in all directions:

scattered waves = spherical isotropic waves.

http://www.webexhibits.org/causesofcolor/images/content/3doubleslit.jpg



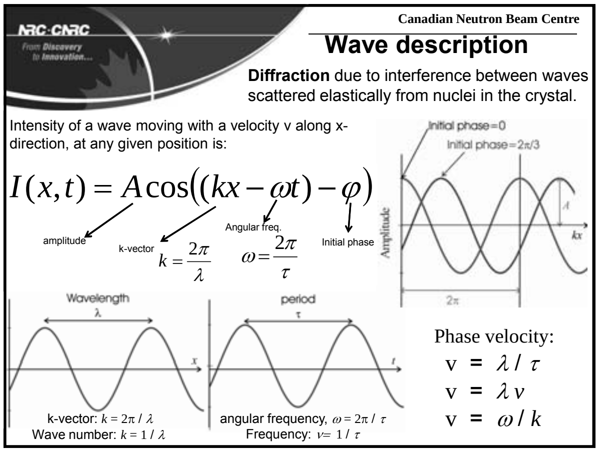
Canadian Neutron Beam Centre

Diffraction: many nuclei in a crystal

Many nuclei: analogy with diffraction of light again:

incident waves = plane waves
nucleus = ideal point scatterer
scattered waves = spherical isotropic waves.

Diffraction due to interference between waves scattered elastically from nuclei in the crystal.



Canadian Neutron Beam Centre

Wave description

Diffraction due to interference between waves scattered elastically from nuclei in the crystal.

Intensity of a wave moving with a velocity v along x-direction, at any given position is:

$$I(x,t) = A\cos\left((kx-\omega t)-\varphi\right)$$

amplitude

k-vector $k=\dfrac{2\pi}{\lambda}$

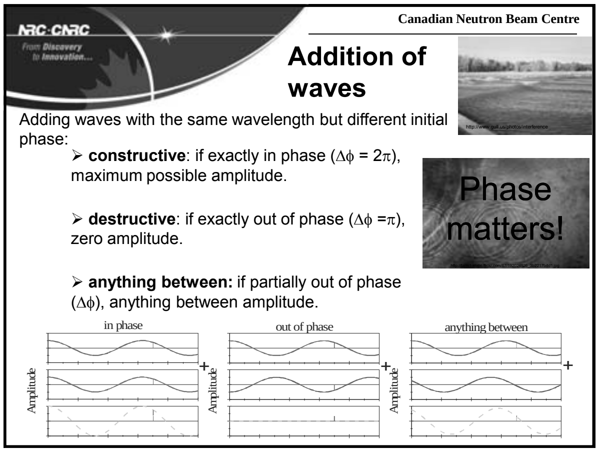
Angular freq. $\omega=\dfrac{2\pi}{\tau}$

Initial phase

k-vector: $k = 2\pi / \lambda$
Wave number: $k = 1 / \lambda$

angular frequency, $\omega = 2\pi / \tau$
Frequency: $\nu = 1 / \tau$

Phase velocity:
$v = \lambda / \tau$
$v = \lambda \nu$
$v = \omega / k$



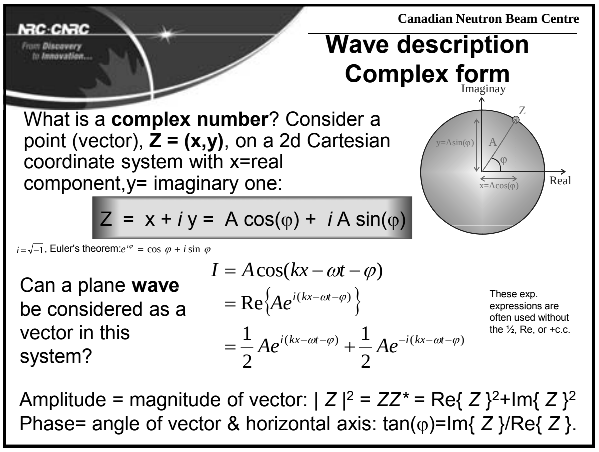
Canadian Neutron Beam Centre

Addition of waves

Phase matters!

Adding waves with the same wavelength but different initial phase:

- **constructive**: if exactly in phase (Δϕ = 2π), maximum possible amplitude.
- **destructive**: if exactly out of phase (Δϕ =π), zero amplitude.
- **anything between:** if partially out of phase (Δϕ), anything between amplitude.



Canadian Neutron Beam Centre

Wave description Complex form

What is a **complex number**? Consider a point (vector), **Z = (x,y)**, on a 2d Cartesian coordinate system with x=real component,y= imaginary one:

Z = x + *i* y = A cos(φ) + *i* A sin(φ)

$i=\sqrt{-1}$, Euler's theorem: $e^{i\varphi} = \cos\varphi + i\sin\varphi$

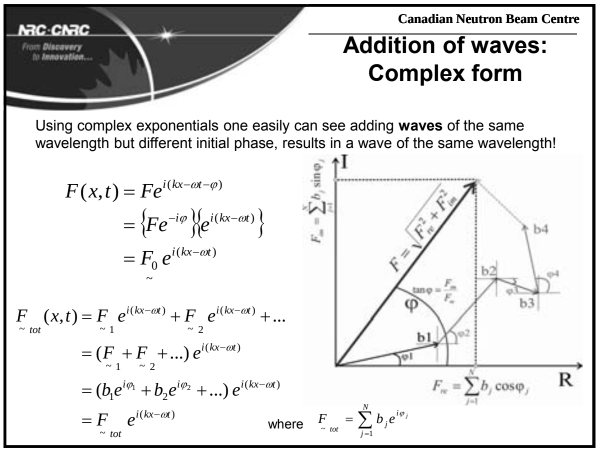
Can a plane **wave** be considered as a vector in this system?

$$I = A\cos(kx-\omega t-\varphi)$$
$$= \mathrm{Re}\left\{Ae^{i(kx-\omega t-\varphi)}\right\}$$
$$= \frac{1}{2}Ae^{i(kx-\omega t-\varphi)} + \frac{1}{2}Ae^{-i(kx-\omega t-\varphi)}$$

These exp. expressions are often used without the ½, Re, or +c.c.

Amplitude = magnitude of vector: $|Z|^2 = ZZ^* = \mathrm{Re}\{Z\}^2 + \mathrm{Im}\{Z\}^2$

Phase= angle of vector & horizontal axis: $\tan(\varphi) = \mathrm{Im}\{Z\}/\mathrm{Re}\{Z\}$.



Canadian Neutron Beam Centre

Addition of waves: Complex form

Using complex exponentials one easily can see adding **waves** of the same wavelength but different initial phase, results in a wave of the same wavelength!

$$F(x,t) = Fe^{i(kx-\omega t-\varphi)}$$
$$= \left\{Fe^{-i\varphi}\right\}\left\{e^{i(kx-\omega t)}\right\}$$
$$= \underset{\sim}{F_0}\, e^{i(kx-\omega t)}$$

$$\underset{\sim}{F}_{tot}(x,t) = \underset{\sim}{F}_1\, e^{i(kx-\omega t)} + \underset{\sim}{F}_2\, e^{i(kx-\omega t)} + \ldots$$
$$= (\underset{\sim}{F}_1 + \underset{\sim}{F}_2 + \ldots)\, e^{i(kx-\omega t)}$$
$$= (b_1 e^{i\varphi_1} + b_2 e^{i\varphi_2} + \ldots)\, e^{i(kx-\omega t)}$$
$$= \underset{\sim}{F}_{tot}\, e^{i(kx-\omega t)}$$

where $\underset{\sim}{F}_{tot} = \sum_{j=1}^{N} b_j e^{i\varphi_j}$

Diffraction from crystals: Bragg's law

Cartoon from Neutron Primer by Roger Pynn, Los Alamos Science (1990)

- Crystals diffract radiation of a similar order of wavelength to the inter-atomic spacings.
- This diffraction is modeled by considering the "reflection" of radiation from equally spaced (d) planes:

Bragg's Law: $2d \sin\theta = n\lambda$

Bragg's law + d-spacing equation $\Longrightarrow$ solve a variety of problems!

Diffraction from crystals: Bragg's law

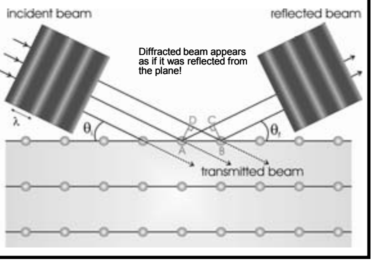
Diffraction from a single layer of atoms: Specular reflection.

Similar to reflection of visible light of a smooth surface like a mirror.

Constructive interference of waves scattered from the two successive lattice points A and B in the plane:

AC = DB

$\theta_i = \theta_f$



Diffracted beam appears as if it was reflected from the plane!

Diffraction from crystals: Bragg's law

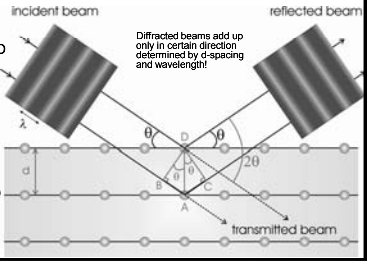
Diffraction: neutrons interact with nuclei → scattered in all directions by every nucleus they encounter. Scattered waves from different nuclei travel different distances → acquire different phase → interfere as they add up!

Constructive interference of waves scattered from two lattice points A and D in adjacent planes:

$$AB + AC = n\lambda$$

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

Bragg's Law

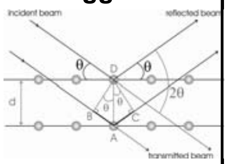


Diffracted beams add up only in certain direction determined by d-spacing and wavelength!

Canadian Neutron Beam Centre

More on Bragg's law

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



- ➢ Diffraction peaks observed only when successive planes scatter in phase (it is relative phase that matters): Coherent scattering from a single plane not sufficient.

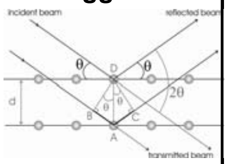
- ➢ For a set of lattice planes diffraction occurs only at a particular angle given by Bragg's law. Larger d-spacing → smaller diffraction angle: inverse relation between d-spacing and q (reciprocal space).

- ➢ No Bragg's scattering when λ is larger than $2d_{max}$ (largest spacing Bragg planes in a material). This is why visible light cannot be used. What is the incident angle for $\lambda=2d_{max}$?

Canadian Neutron Beam Centre

More on Bragg's law

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



- ➢ Planes must pass through same points in all the unit cells in the crystal to diffract in phase. Only if planes cut all the 3 cell edges an integral number of times, unit cells diffract in phase.

- ➢ Miller indices used to label the planes: $d_{nhnknl} = \frac{d_{hkl}}{n}$ → $2d_{hkl} \sin\theta = \lambda$. Only need to consider the n=1 values, since higher values of n for the (hkl) planes correspond to the n=1 value for the (nh nk nl) planes.

- ➢ Plane of "reflection" bisects the angle between incident and scattered beams: 2θ is measured in experiment. Either (a) rotate the sample (single crystal) or (b) have lots of crystals at different orientations simultaneously (powder).

Canadian Neutron Beam Centre

Mathematical foundation of neutron scattering

Reminder: **neutron** can be thought about as a **wave**! described by a **wavefunction, ψ.**

Probability of finding a neutron at a given point in space

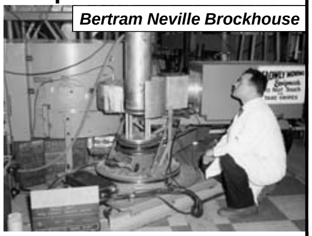
$$|\psi|^2 = \psi \times \psi^*$$

Neutron wavevector $\mathbf{k}$: a vector pointing along neutron's trajectory.

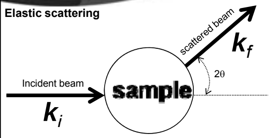
Wavevector magnitude: $k = |\mathbf{k}| = \frac{2\pi}{\lambda} = 2\pi\, mv\, h.$

Canadian Neutron Beam Centre

How is it related to experiment?


Bertram Neville Brockhouse

Elastic scattering



Scattering vector

$$Q = k_i - k_f$$

Conservation of momentum

Momentum transfer= ħ**Q** with |**Q**|= Q=4π sinθ/λ

The **number of scattered neutrons** as a function of **Q** is measured. The result is the scattering function S(**Q**) depending only on the properties of the sample.

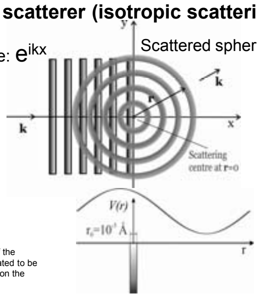
Canadian Neutron Beam Centre

Scattering by a fixed single nucleus

Neutrons interact with matter via nuclear force: very short range ~10^{-15} m, size of a nucleus ~100,000 times smaller than distance between centers!
Nucleus → **point scatterer (isotropic scattering)!**

Incident plane wave: e^{ikx}

Scattered spherical wave: $-\frac{b}{r}e^{ikr}$



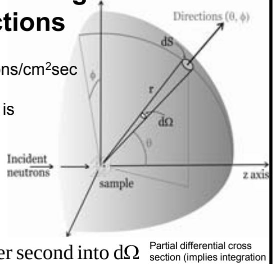
Squared modulus =1 anywhere, neutron is found with same probability at all positions!

Squared modulus=b^2/r^2, neutron is found with same probability in any direction but with amplitude b/r: b is scattering length (n-N interaction strength),1/r to account for 1/r2 decrease in intensity as scattered wavefront grows in size with r.

The spatial extent of the potential is exaggerated to be able to show it here on the same scale!

Canadian Neutron Beam Centre

Scattering cross sections



Incident flux: Φ=number of incident neutrons/cm^{2}sec

Incident neutron beam directed along polar is scattered by the sample along (θ, ϕ).

Detector measures all the neutrons into solid angle dΩ in the direction of (θ, ϕ).

Differential cross-section:

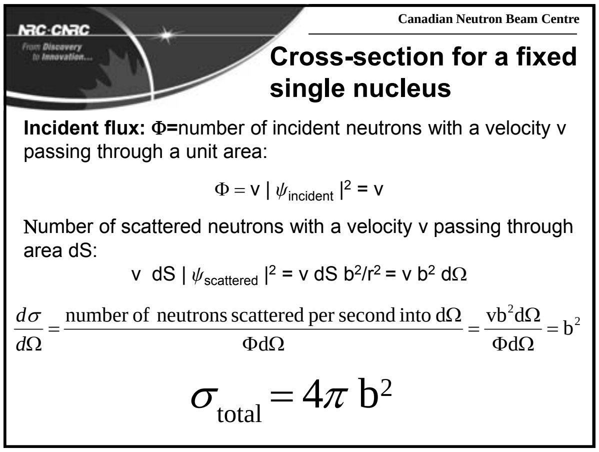
$$\frac{d\sigma}{d\Omega} = \frac{\text{number of neutrons scattered per second into d}\Omega}{\Phi \text{d}\Omega}$$

Partial differential cross section (implies integration over all energies or no energy analysis).

Total cross section:

$$\sigma = \int_0^{4\pi} \frac{d\sigma}{d\Omega} d\Omega = \frac{\text{total number of neutrons scattered per second}}{\Phi}$$

Total number of scattered neutrons in all directions (units: barn=10^{-24} cm^2)



Canadian Neutron Beam Centre

Cross-section for a fixed single nucleus

Incident flux: Φ=number of incident neutrons with a velocity v passing through a unit area:

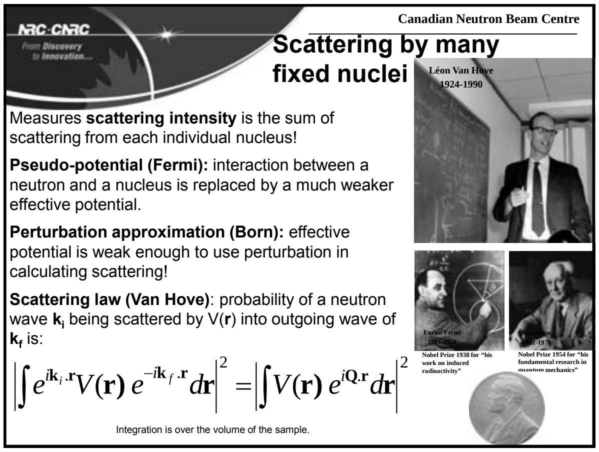
$$\Phi = v\,|\psi_{\text{incident}}|^2 = v$$

Number of scattered neutrons with a velocity v passing through area dS:

$$v\ dS\,|\psi_{\text{scattered}}|^2 = v\,dS\,b^2/r^2 = v\,b^2\,d\Omega$$

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

$$\sigma_{\text{total}} = 4\pi\,b^2$$



Canadian Neutron Beam Centre

Scattering by many fixed nuclei

Measures **scattering intensity** is the sum of scattering from each individual nucleus!

Pseudo-potential (Fermi): interaction between a neutron and a nucleus is replaced by a much weaker effective potential.

Perturbation approximation (Born): effective potential is weak enough to use perturbation in calculating scattering!

Scattering law (Van Hove): probability of a neutron wave $\mathbf{k}_i$ being scattered by V(**r**) into outgoing wave of $\mathbf{k}_f$ is:

$$\left|\int e^{i\mathbf{k}_i.\mathbf{r}} V(\mathbf{r})\, e^{-i\mathbf{k}_f.\mathbf{r}} d\mathbf{r}\right|^2 = \left|\int V(\mathbf{r})\, e^{i\mathbf{Q}.\mathbf{r}} d\mathbf{r}\right|^2$$

Integration is over the volume of the sample.

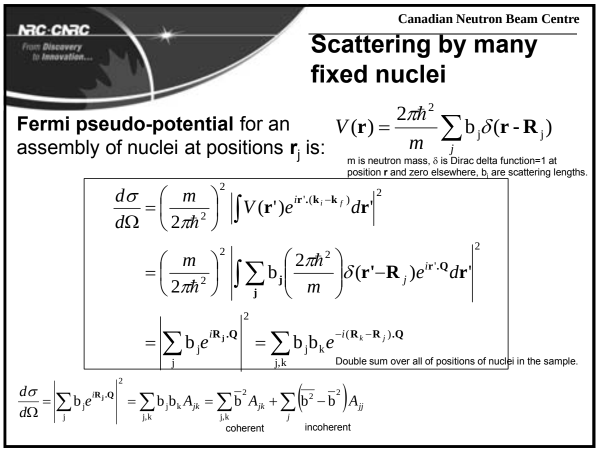
Léon Van Hove
1924-1990

Enrico Fermi
1901-1954

Nobel Prize 1938 for "his work on induced radioactivity"

Max Born
1882-1970

Nobel Prize 1954 for "his fundamental research in quantum mechanics"



Canadian Neutron Beam Centre

Scattering by many fixed nuclei

Fermi pseudo-potential for an assembly of nuclei at positions $\mathbf{r}_j$ is:

$$V(\mathbf{r}) = \frac{2\pi\hbar^2}{m}\sum_j b_j\delta(\mathbf{r} - \mathbf{R}_j)$$

m is neutron mass, δ is Dirac delta function=1 at position **r** and zero elsewhere, b_j are scattering lengths.

$$\boxed{\begin{aligned}\frac{d\sigma}{d\Omega} &= \left(\frac{m}{2\pi\hbar^2}\right)^2 \left|\int V(\mathbf{r}')e^{i\mathbf{r}'.(\mathbf{k}_i-\mathbf{k}_f)}d\mathbf{r}'\right|^2 \\ &= \left(\frac{m}{2\pi\hbar^2}\right)^2 \left|\int\sum_{\mathbf{j}} b_{\mathbf{j}}\left(\frac{2\pi\hbar^2}{m}\right)\delta(\mathbf{r}'-\mathbf{R}_j)e^{i\mathbf{r}'.\mathbf{Q}}d\mathbf{r}'\right|^2 \\ &= \left|\sum_j b_j e^{i\mathbf{R}_j.\mathbf{Q}}\right|^2 = \sum_{j,k} b_j b_k e^{-i(\mathbf{R}_k-\mathbf{R}_j).\mathbf{Q}}\end{aligned}}$$

Double sum over all of positions of nuclei in the sample.

$$\frac{d\sigma}{d\Omega} = \left|\sum_j b_j e^{i\mathbf{R}_j.\mathbf{Q}}\right|^2 = \sum_{j,k} b_j b_k A_{jk} = \underbrace{\sum_{j,k}\bar{b}^2 A_{jk}}_{\text{coherent}} + \underbrace{\sum_j\left(\overline{b^2}-\bar{b}^2\right)A_{jj}}_{\text{incoherent}}$$

Canadian Neutron Beam Centre

More on scattering by many fixed nuclei

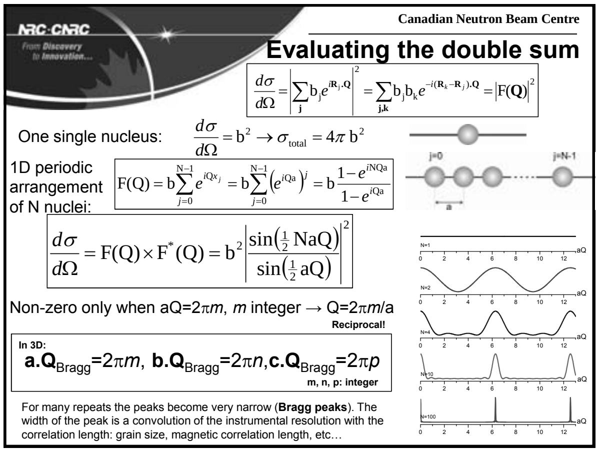
$$\frac{d\sigma}{d\Omega} = \sum_{\mathbf{j,k}} \mathrm{b_j b_k}\, e^{-i(\mathbf{R}_k - \mathbf{R}_j).\mathbf{Q}} = \sum_{\mathbf{j,k}} \mathrm{b_j b_k} \int_{-\infty}^{\infty} \delta(\mathbf{r} - (\mathbf{R}_j - \mathbf{R}_k))\, e^{-i\mathbf{r}.\mathbf{Q}}\, \mathrm{d}\mathbf{r}$$

For $b_j = b_k$:

$$\boxed{\begin{gathered}\frac{d\sigma}{d\Omega} = \mathrm{N\, b}^2 \int_{-\infty}^{\infty} \mathrm{G}(\mathbf{r})\, e^{-i\mathbf{r}.\mathbf{Q}}\, \mathrm{d}\mathbf{r} \\ \mathrm{G}(\mathbf{r}) = \frac{1}{\mathrm{N}} \sum_{j,k} \delta(\mathbf{r} - (\mathbf{R}_j - \mathbf{R}_k))\end{gathered}}$$

Fourier transform of pair correlation function G(**r**)

Intensity is proportional to **Fourier transform** of **pair correlation function** (probability of finding two atoms being a certain distance apart). Scattering gives information about correlations between positions of pairs of nuclei.



Canadian Neutron Beam Centre

Evaluating the double sum

$$\boxed{\frac{d\sigma}{d\Omega} = \left|\sum_{\mathbf{j}} \mathrm{b_j} e^{i\mathbf{R}_j.\mathbf{Q}}\right|^2 = \sum_{\mathbf{j,k}} \mathrm{b_j b_k} e^{-i(\mathbf{R}_k - \mathbf{R}_j).\mathbf{Q}} = |\mathrm{F}(\mathbf{Q})|^2}$$

One single nucleus: $\frac{d\sigma}{d\Omega} = \mathrm{b}^2 \rightarrow \sigma_{\mathrm{total}} = 4\pi\, \mathrm{b}^2$

1D periodic arrangement of N nuclei: $\boxed{\mathrm{F(Q)} = \mathrm{b}\sum_{j=0}^{\mathrm{N}-1} e^{i\mathrm{Q}x_j} = \mathrm{b}\sum_{j=0}^{\mathrm{N}-1}\left(e^{i\mathrm{Qa}}\right)^j = \mathrm{b}\frac{1-e^{i\mathrm{NQa}}}{1-e^{i\mathrm{Qa}}}}$

$$\boxed{\frac{d\sigma}{d\Omega} = \mathrm{F(Q)} \times \mathrm{F}^*(\mathrm{Q}) = \mathrm{b}^2 \left|\frac{\sin\left(\frac{1}{2}\mathrm{NaQ}\right)}{\sin\left(\frac{1}{2}\mathrm{aQ}\right)}\right|^2}$$

Non-zero only when aQ=2π*m*, *m* integer → Q=2π*m*/a

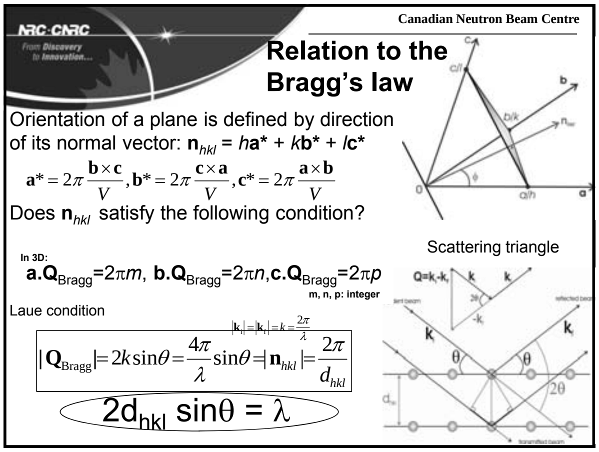
Reciprocal!

In 3D:

a.Q$_{\mathrm{Bragg}}$=2π*m*, **b.Q**$_{\mathrm{Bragg}}$=2π*n*,**c.Q**$_{\mathrm{Bragg}}$=2π*p*

m, n, p: integer

For many repeats the peaks become very narrow (**Bragg peaks**). The width of the peak is a convolution of the instrumental resolution with the correlation length: grain size, magnetic correlation length, etc…



Canadian Neutron Beam Centre

Relation to the Bragg's law

Orientation of a plane is defined by direction of its normal vector: **n**$_{hkl}$ = *h***a*** + *k***b*** + *l***c***

$$\mathbf{a}^* = 2\pi\frac{\mathbf{b}\times\mathbf{c}}{V}, \mathbf{b}^* = 2\pi\frac{\mathbf{c}\times\mathbf{a}}{V}, \mathbf{c}^* = 2\pi\frac{\mathbf{a}\times\mathbf{b}}{V}$$

Does **n**$_{hkl}$ satisfy the following condition?

In 3D:

a.Q$_{\mathrm{Bragg}}$=2π*m*, **b.Q**$_{\mathrm{Bragg}}$=2π*n*,**c.Q**$_{\mathrm{Bragg}}$=2π*p*

m, n, p: integer

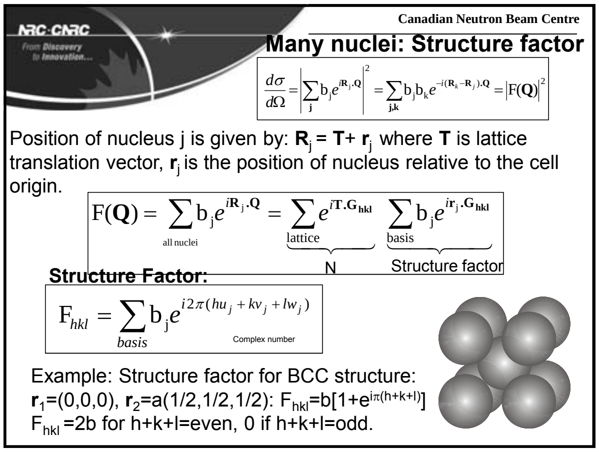
Laue condition

$$|\mathbf{k}_i| = |\mathbf{k}_f| = k = \frac{2\pi}{\lambda}$$

$$\boxed{|\mathbf{Q}_{\mathrm{Bragg}}| = 2k\sin\theta = \frac{4\pi}{\lambda}\sin\theta = |\mathbf{n}_{hkl}| = \frac{2\pi}{d_{hkl}}}$$

$2\mathrm{d}_{\mathrm{hkl}} \sin\theta = \lambda$

Scattering triangle



Canadian Neutron Beam Centre

Many nuclei: Structure factor

$$\frac{d\sigma}{d\Omega} = \left|\sum_{\mathbf{j}} \mathrm{b_j} e^{i\mathbf{R}_j.\mathbf{Q}}\right|^2 = \sum_{\mathbf{j,k}} \mathrm{b_j b_k} e^{-i(\mathbf{R}_k-\mathbf{R}_j).\mathbf{Q}} = |\mathrm{F}(\mathbf{Q})|^2$$

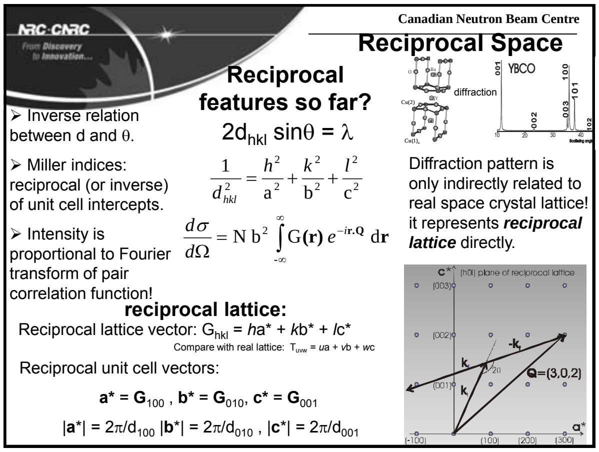
Position of nucleus j is given by: $\mathbf{R}_j = \mathbf{T} + \mathbf{r}_j$ where **T** is lattice translation vector, $\mathbf{r}_j$ is the position of nucleus relative to the cell origin.

$$\mathrm{F}(\mathbf{Q}) = \sum_{\text{all nuclei}} \mathrm{b_j} e^{i\mathbf{R}_j.\mathbf{Q}} = \underbrace{\sum_{\text{lattice}} e^{i\mathbf{T}.\mathbf{G}_{\mathbf{hkl}}}}_{\text{N}} \underbrace{\sum_{\text{basis}} \mathrm{b_j} e^{i\mathbf{r}_j.\mathbf{G}_{\mathbf{hkl}}}}_{\text{Structure factor}}$$

Structure Factor:

$$\mathrm{F}_{hkl} = \sum_{basis} \mathrm{b_j} e^{i2\pi(hu_j+kv_j+lw_j)} \quad \text{Complex number}$$

Example: Structure factor for BCC structure:
$\mathbf{r}_1$=(0,0,0), $\mathbf{r}_2$=a(1/2,1/2,1/2): $\mathrm{F_{hkl}}=\mathrm{b}[1+e^{i\pi(h+k+l)}]$
$\mathrm{F_{hkl}}$ =2b for h+k+l=even, 0 if h+k+l=odd.



Canadian Neutron Beam Centre

Reciprocal Space

Reciprocal features so far?

- Inverse relation between d and θ.

$$2\mathrm{d_{hkl}}\sin\theta = \lambda$$

- Miller indices: reciprocal (or inverse) of unit cell intercepts.

$$\frac{1}{d_{hkl}^2} = \frac{h^2}{\mathrm{a}^2} + \frac{k^2}{\mathrm{b}^2} + \frac{l^2}{\mathrm{c}^2}$$

- Intensity is proportional to Fourier transform of pair correlation function!

$$\frac{d\sigma}{d\Omega} = \mathrm{N\,b}^2 \int_{-\infty}^{\infty} \mathrm{G}(\mathbf{r})\, e^{-i\mathbf{r}.\mathbf{Q}}\, \mathrm{d}\mathbf{r}$$

Diffraction pattern is only indirectly related to real space crystal lattice! it represents ***reciprocal lattice*** directly.

reciprocal lattice:

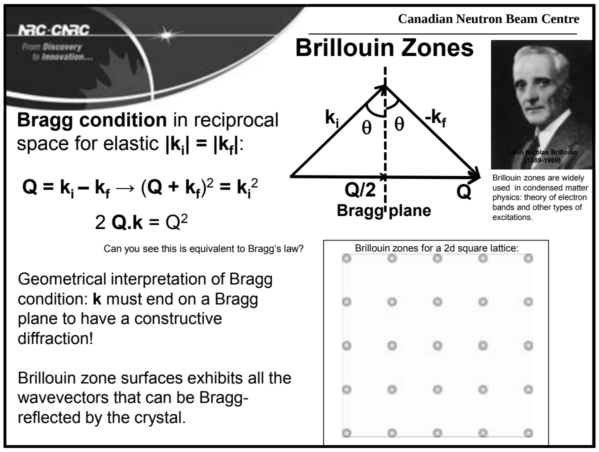
Reciprocal lattice vector: $\mathrm{G_{hkl}} = h\mathrm{a}^* + k\mathrm{b}^* + l\mathrm{c}^*$

Compare with real lattice: $\mathrm{T_{uvw}} = u\mathrm{a} + v\mathrm{b} + w\mathrm{c}$

Reciprocal unit cell vectors:

$$\mathbf{a}^* = \mathbf{G}_{100}\ ,\ \mathbf{b}^* = \mathbf{G}_{010},\ \mathbf{c}^* = \mathbf{G}_{001}$$

$$|\mathbf{a}^*| = 2\pi/\mathrm{d}_{100}\ |\mathbf{b}^*| = 2\pi/\mathrm{d}_{010}\ ,\ |\mathbf{c}^*| = 2\pi/\mathrm{d}_{001}$$



Canadian Neutron Beam Centre

Brillouin Zones

Bragg condition in reciprocal space for elastic $|\mathbf{k}_i| = |\mathbf{k}_f|$:

$$\mathbf{Q} = \mathbf{k}_i - \mathbf{k}_f \rightarrow (\mathbf{Q} + \mathbf{k}_f)^2 = \mathbf{k}_i^2$$

$$2\,\mathbf{Q}.\mathbf{k} = \mathrm{Q}^2$$

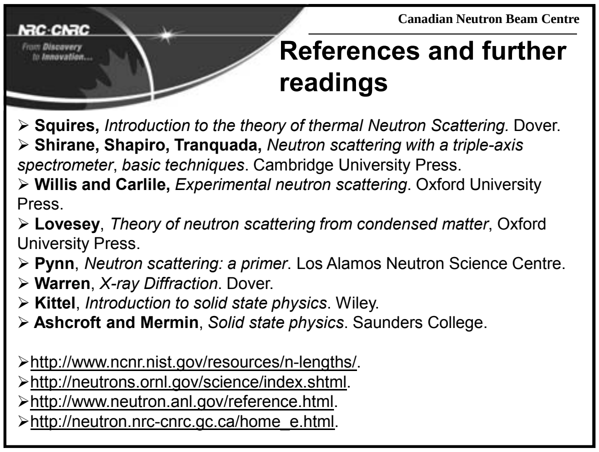
Can you see this is equivalent to Bragg's law?

Brillouin zones are widely used in condensed matter physics: theory of electron bands and other types of excitations.

Geometrical interpretation of Bragg condition: **k** must end on a Bragg plane to have a constructive diffraction!

Brillouin zone surfaces exhibits all the wavevectors that can be Bragg-reflected by the crystal.

Brillouin zones for a 2d square lattice:



Canadian Neutron Beam Centre

References and further readings

- **Squires,** *Introduction to the theory of thermal Neutron Scattering.* Dover.
- **Shirane, Shapiro, Tranquada,** *Neutron scattering with a triple-axis spectrometer*, *basic techniques*. Cambridge University Press.
- **Willis and Carlile,** *Experimental neutron scattering*. Oxford University Press.
- **Lovesey**, *Theory of neutron scattering from condensed matter*, Oxford University Press.
- **Pynn**, *Neutron scattering: a primer*. Los Alamos Neutron Science Centre.
- **Warren**, *X-ray Diffraction*. Dover.
- **Kittel**, *Introduction to solid state physics*. Wiley.
- **Ashcroft and Mermin**, *Solid state physics*. Saunders College.

- http://www.ncnr.nist.gov/resources/n-lengths/.
- http://neutrons.ornl.gov/science/index.shtml.
- http://www.neutron.anl.gov/reference.html.
- http://neutron.nrc-cnrc.gc.ca/home_e.html.