NRC·CNRC

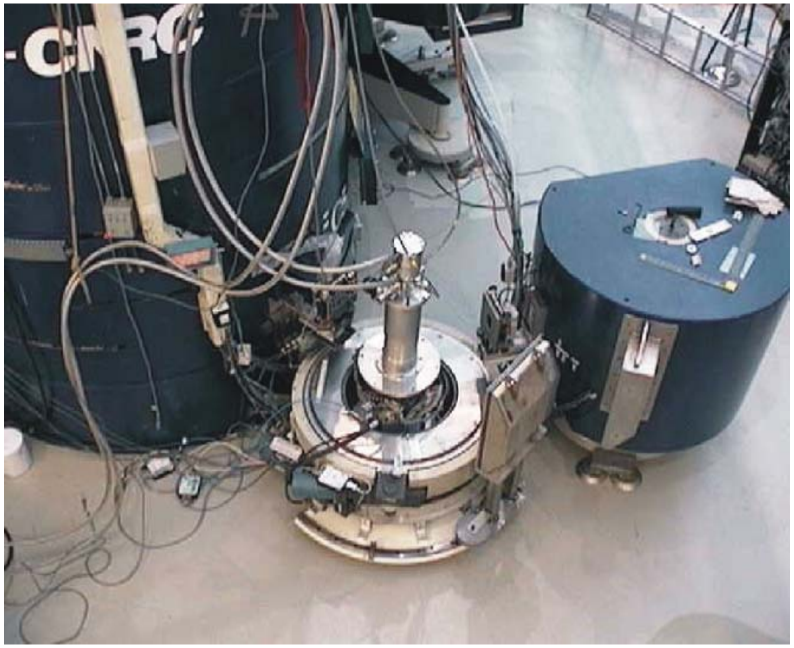
From **Discovery** to **Innovation...**

Neutron Scattering Basics I

Zahra Yamani

NRC - Canadian Neutron Beam Centre, Chalk River, Canada

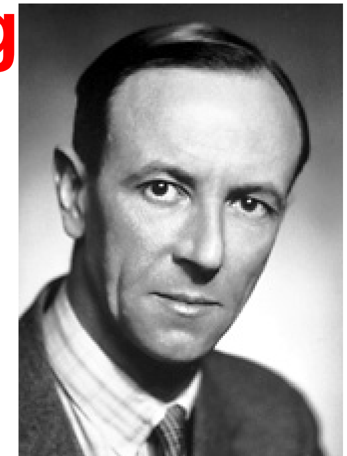
Overview



- 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!

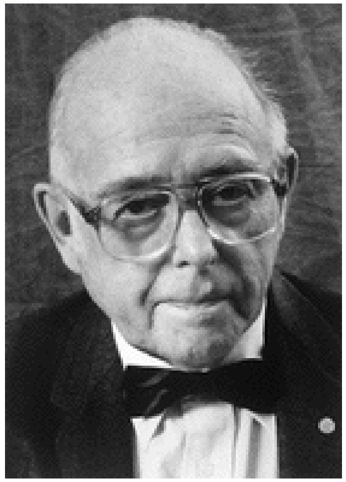
Neutron scattering



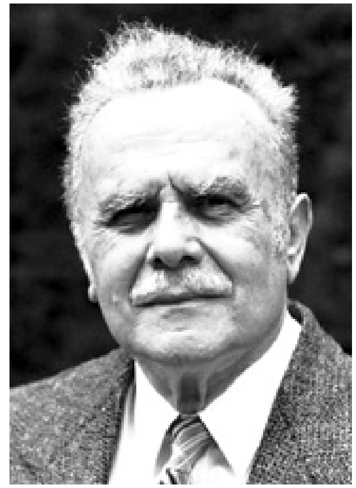
James Chadwick
1891-1974
Nobel Prize 1935 for "the discovery of the neutron"

Nobel Prize 1994

"for the development of the neutron diffraction technique"



Clifford Schull
1915-2001

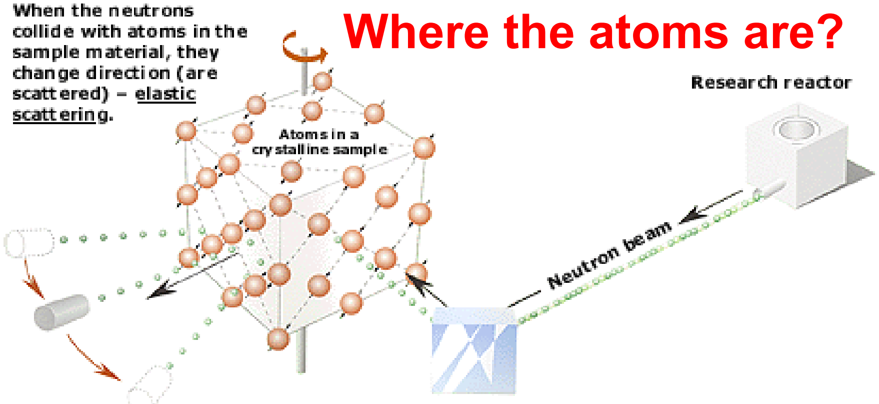


Bertram Brockhouse
1918-2003

"for the development of neutron spectroscopy"

Where the atoms are?

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

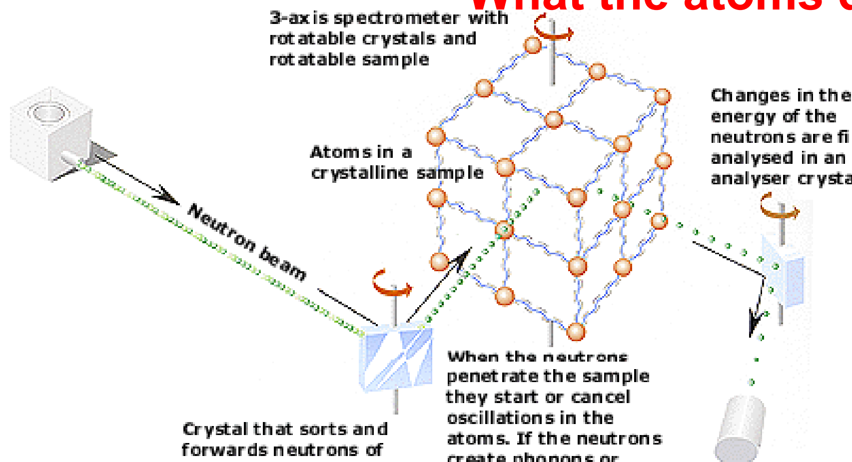


Detectors record the directions of the neutrons and a diffraction pattern is obtained.
The pattern shows the positions of the atoms relative to one another.

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

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

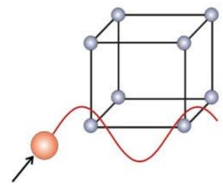
When the neutrons penetrate the sample they start or cancel oscillations in the atoms. If the neutrons create phonons or magnons they themselves lose the energy these absorb – inelastic scattering

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

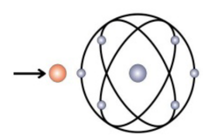
Why neutrons?

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

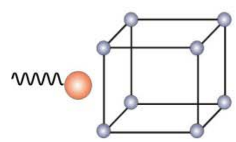
Neutrons are **neutral** particles. They
- are highly penetrating
- can be used as nondestructive probes, and
- can be used to study samples in severe environments



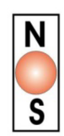
The **wavelengths** of neutrons are similar to atomic spacing. They can determine
- crystal structures and atomic spacing, and
- other structural information.



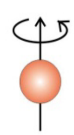
Neutrons “see” **nuclei**. They
- are sensitive to light atoms.
- can exploit isotopic substitution, and
- can use contrast variation to differentiate complex molecular structures.



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.



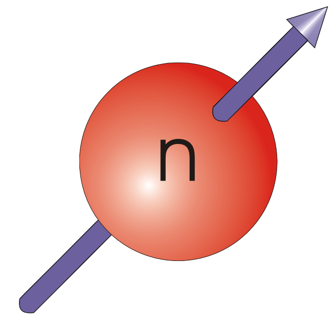
Neutrons have a **magnetic moment**. They can be used to study
- microscopic magnetic structure, and
- study magnetic fluctuations.



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

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)

Crystal Structure

What is a crystal?

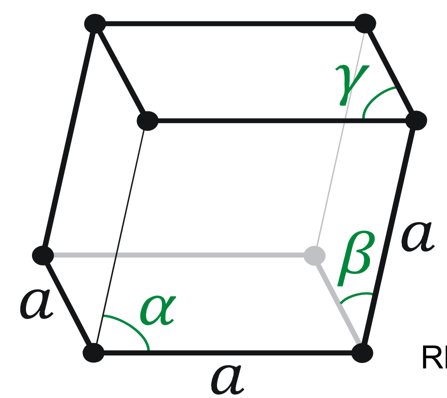
A three dimensional periodic array of atoms.

An ideal crystal ≡ infinite repetition of identical structural units (single atom or compromise many atoms or 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.

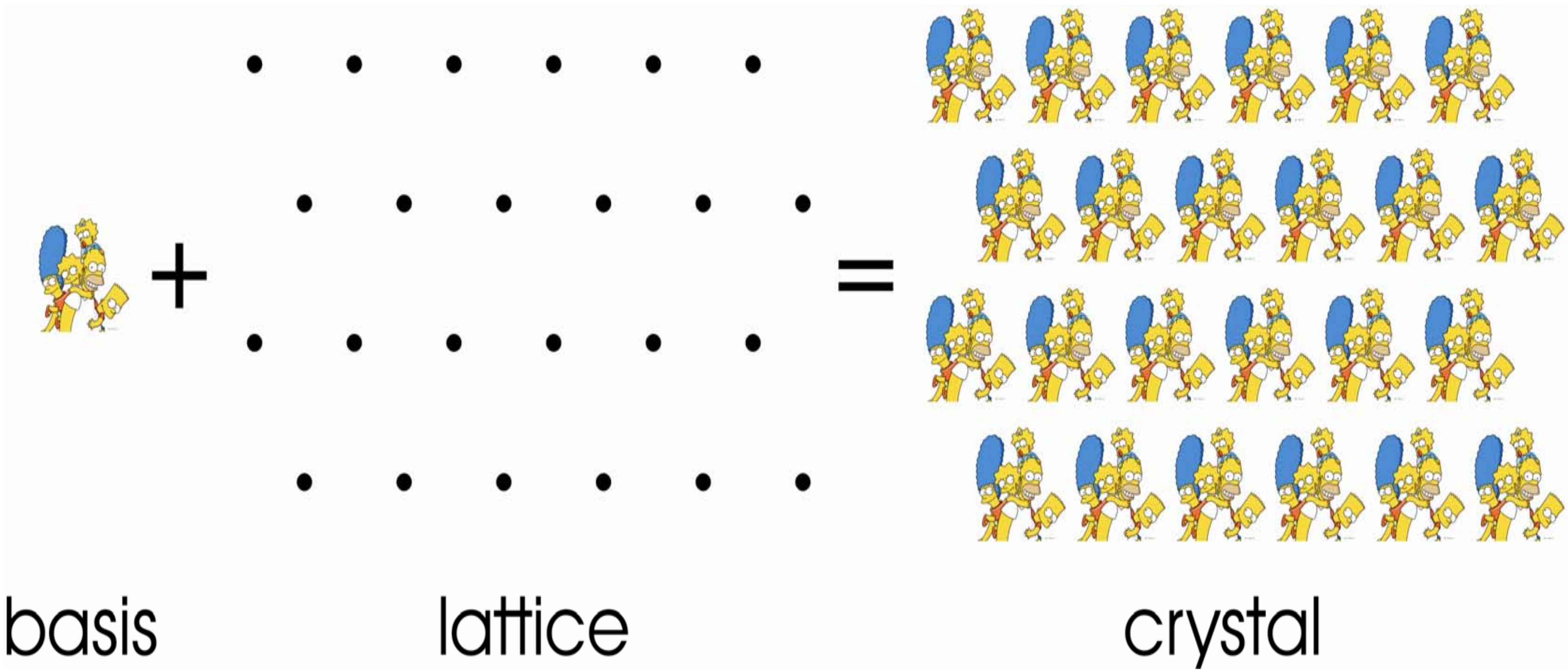
http://www.10xminerals.com/specimens/mineral-specimens.html

$\alpha, \beta, \gamma \neq 90°$



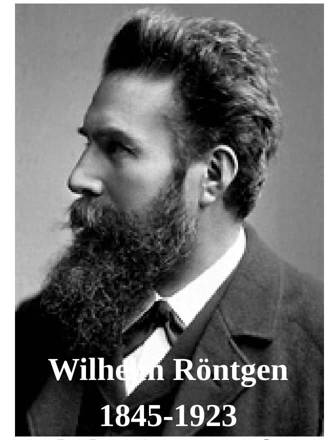
Rhombohedral

Crystal Structure



Why study crystal structures?

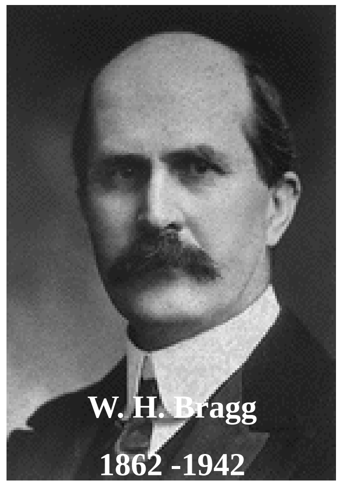
Solid state physics: crystals and electrons in crystals

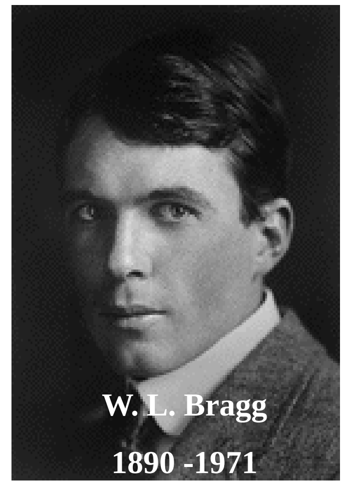


Nobel Prize 1901 for "his discovery of x-rays."

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"



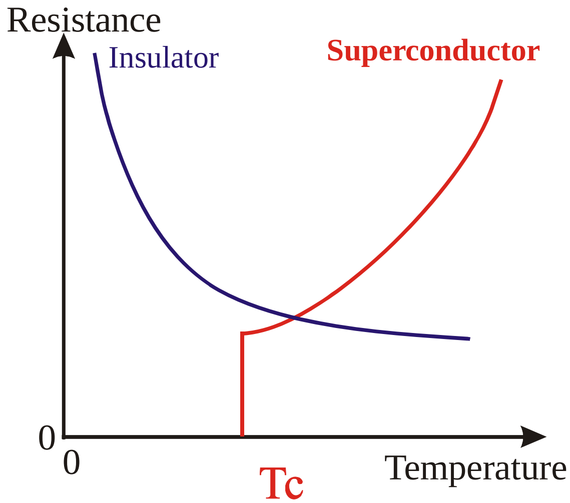


Nobel Prize 1915 "for their services in the analysis of crystal structure by means of X-rays"

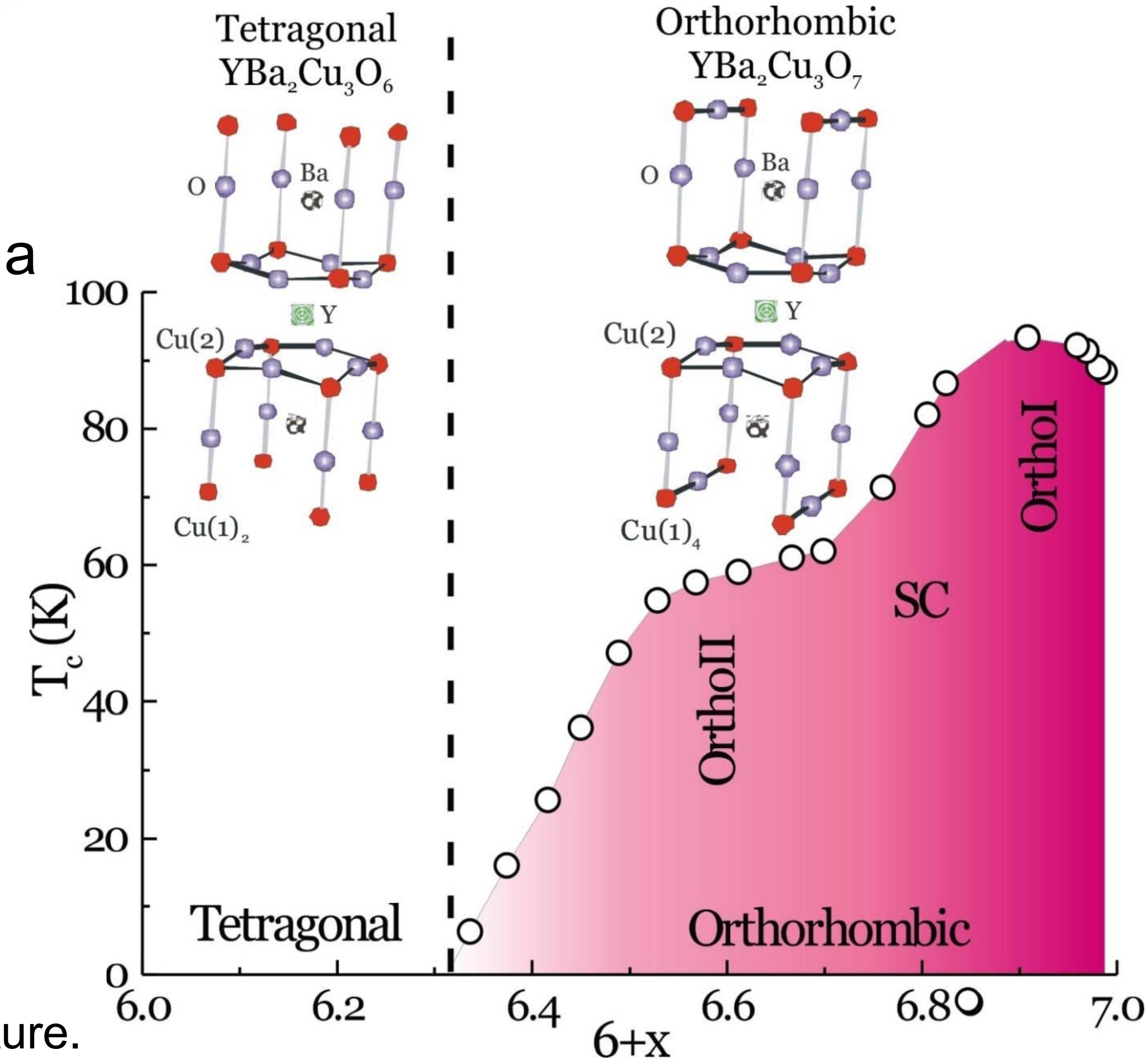
- **to describe solids**
- **be able to compare materials**
- **to predict physical properties**

Why study crystal structures?
An example: HTSC

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



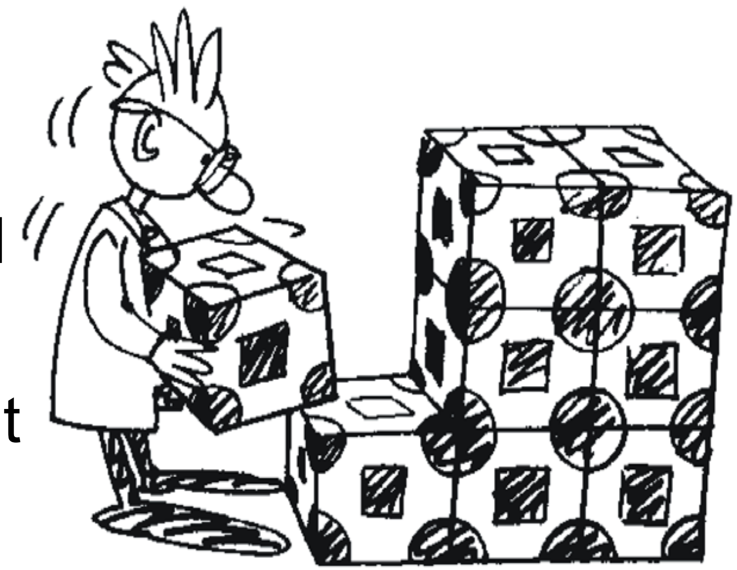
Physical properties are correlated with crystal structure.



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.

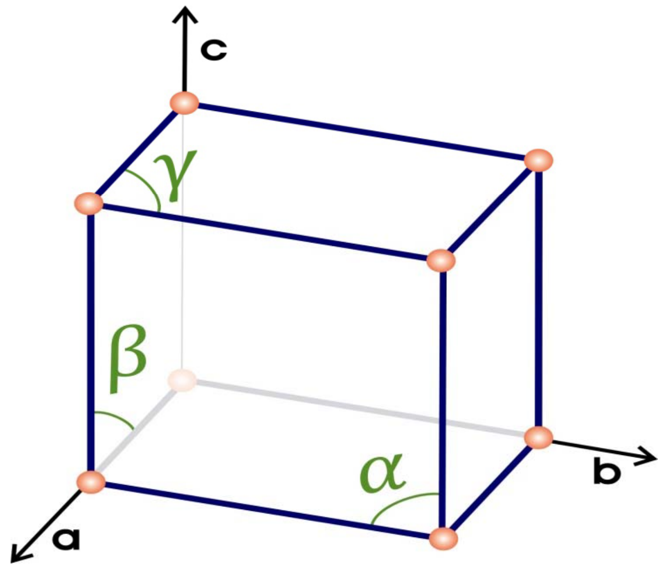


Cartoon from: Neutron Scattering - A primer by Roger Pynn

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.



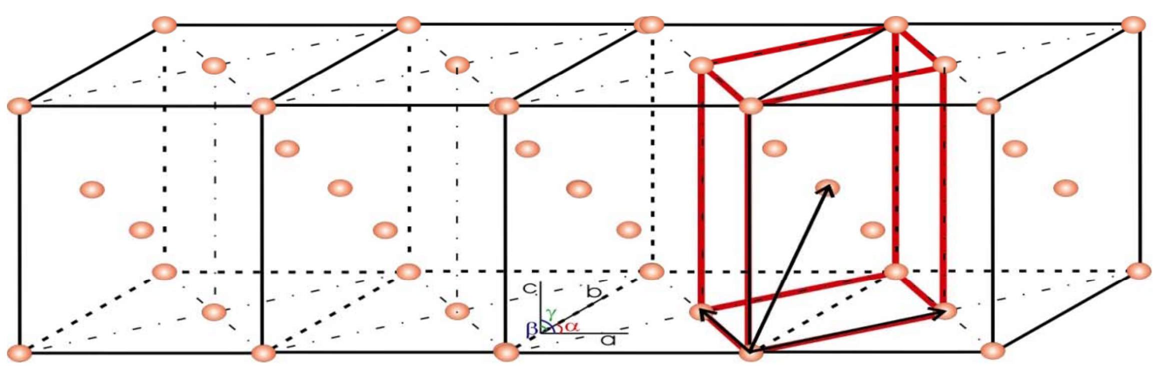
Unit Cell

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

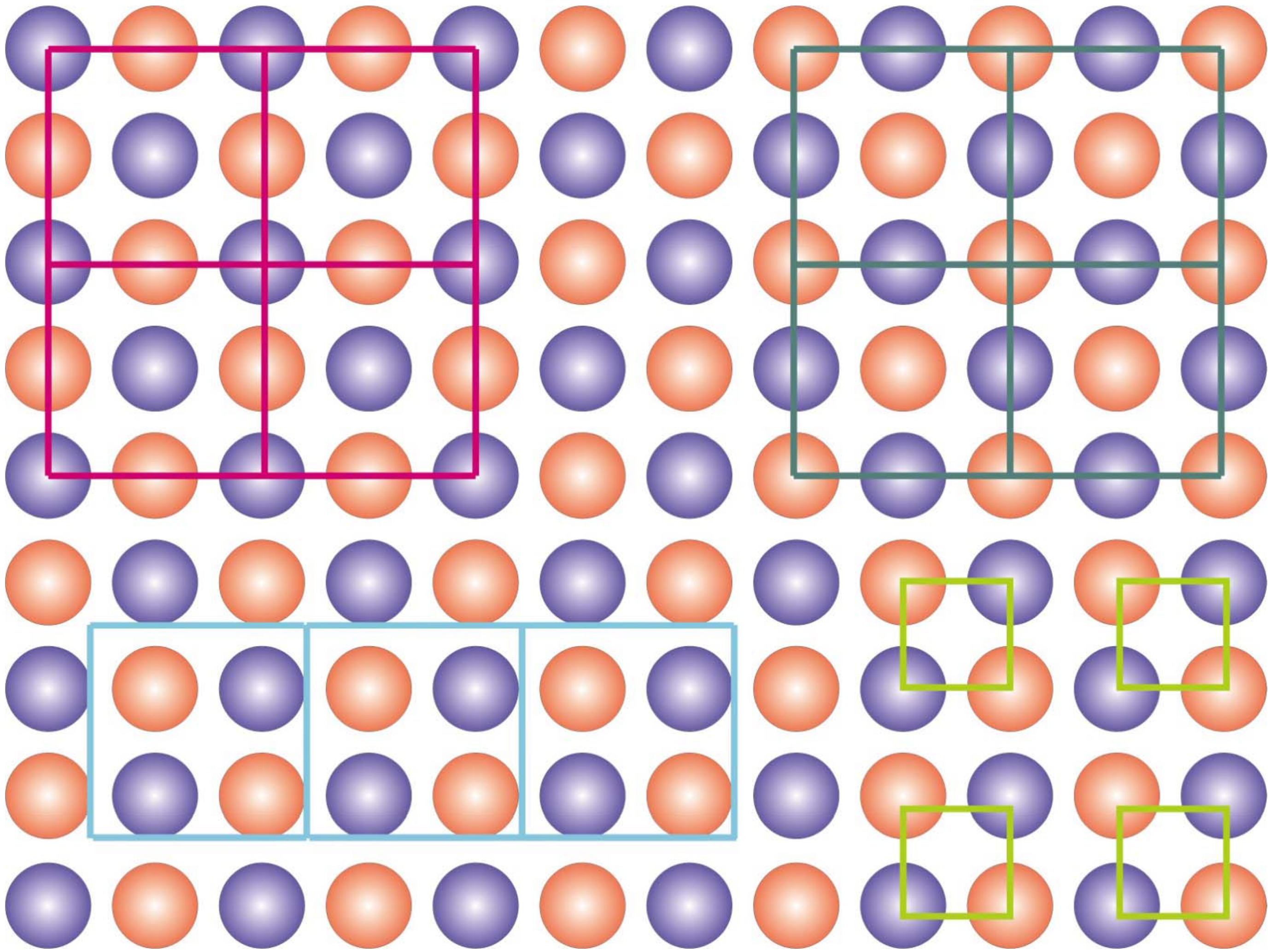
Primitive unit cell = minimum-volume cell when stacked completely fills the space, not always displays all symmetries in the crystal.

An example: fcc crystal

Unit cell = fcc
Primitive cell = bcc



Unit Cell: more examples



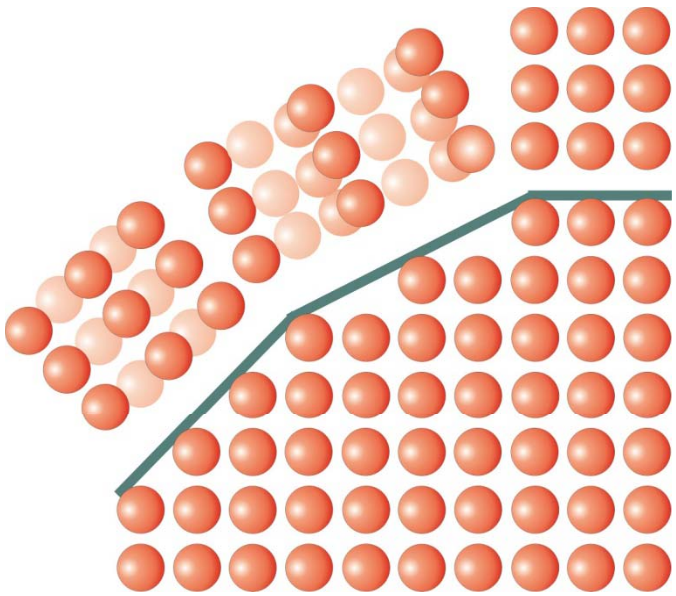
Lattice planes & Miller indices

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.

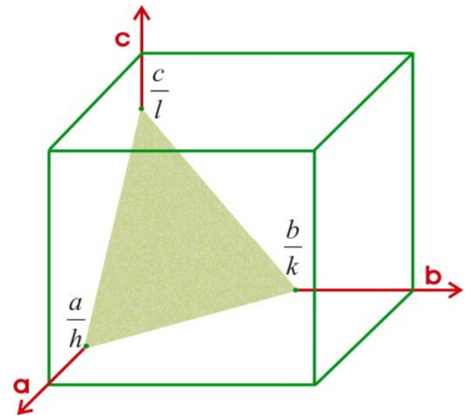


All planes in one direction are identical.

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

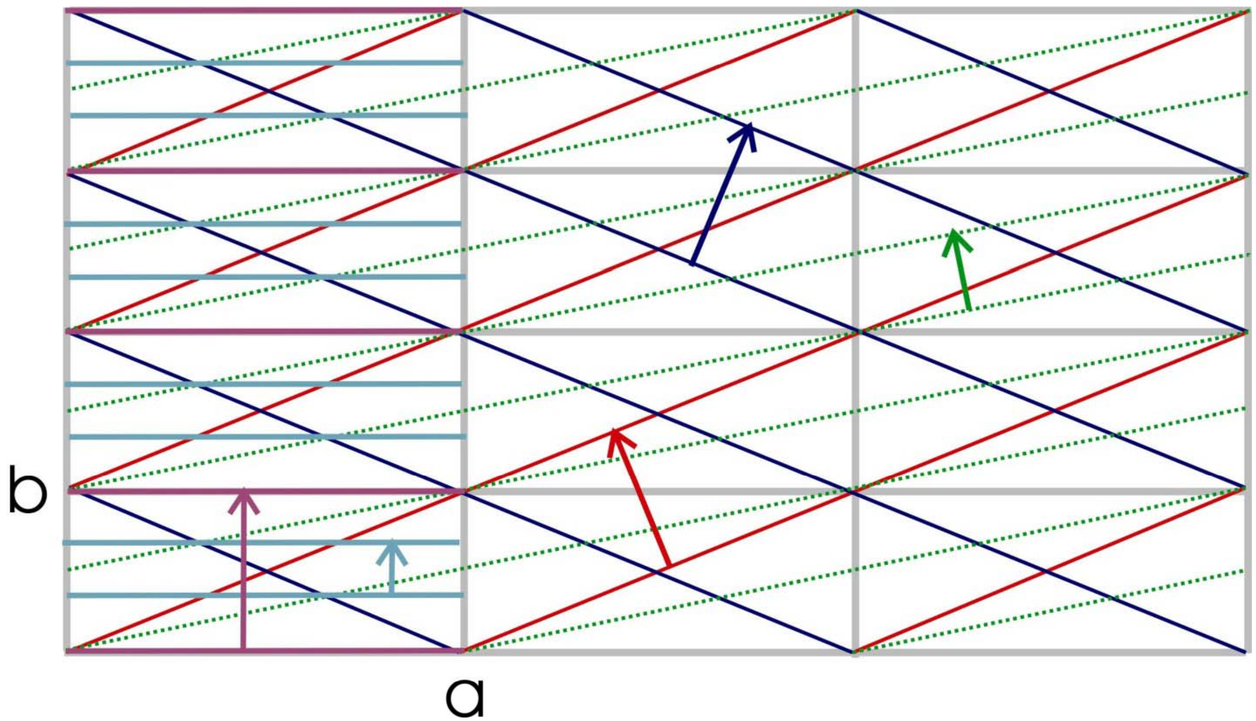
h, k, l

Miller indices

reciprocals of fractional intercepts

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**)!

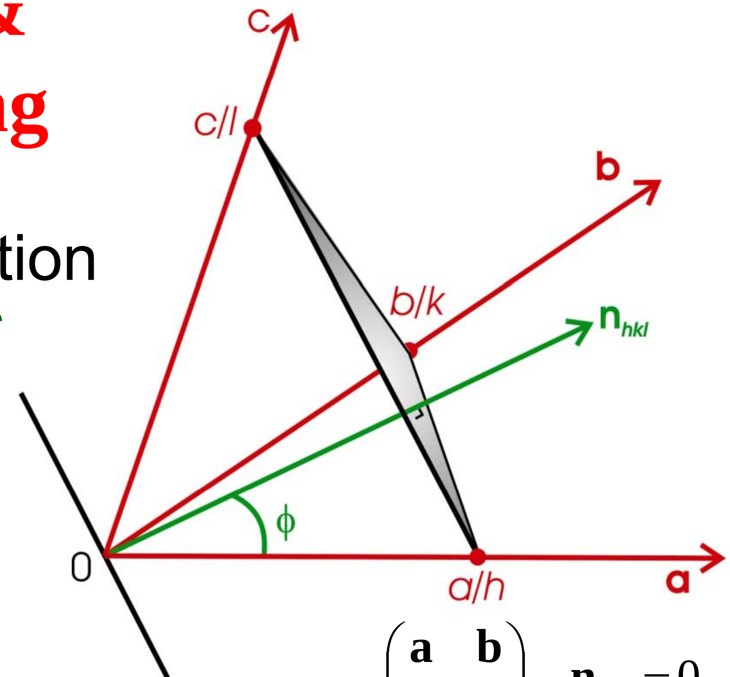
Planes & d-spacing

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

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

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

a*. **a** = 1, **a***. **b** = 0, what about **a***. **c** = ?



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

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

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

What about Triclinic?!

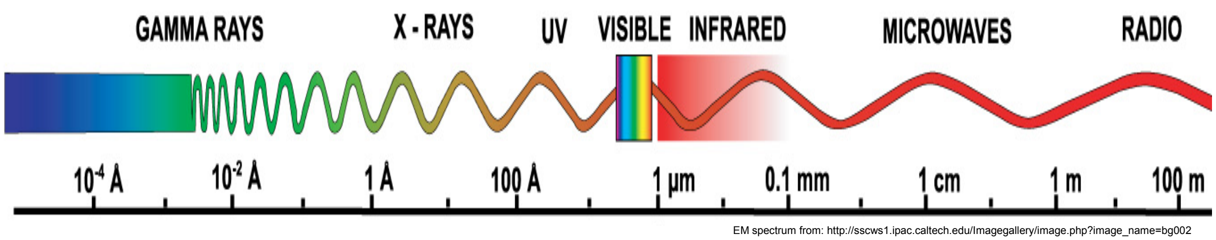
Diffraction

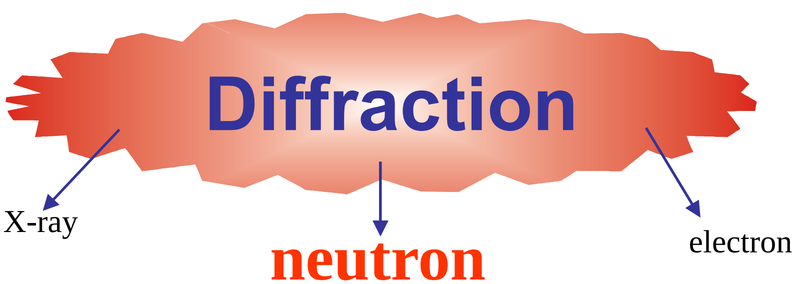
How to determine crystal structure?

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?

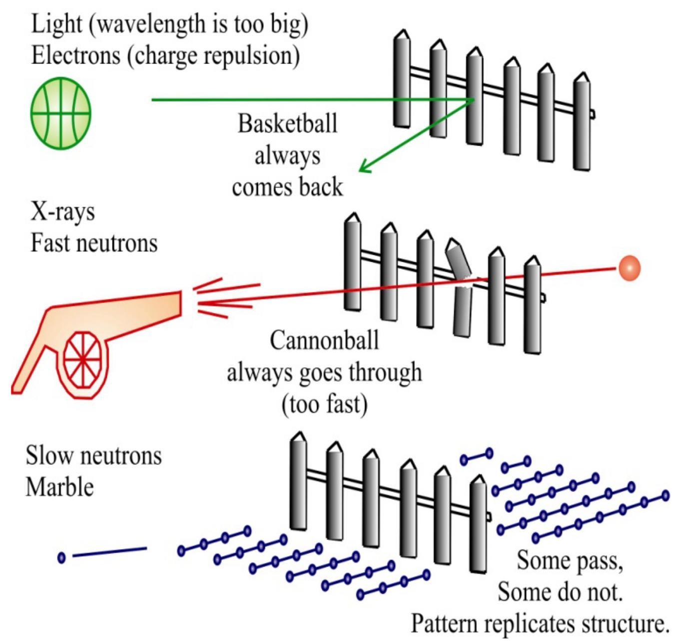




Can be done with X-rays, electrons and neutrons!

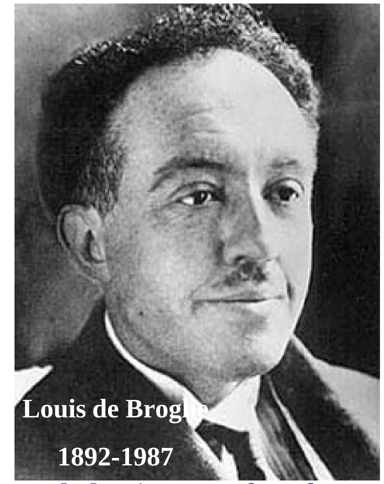
How does neutron scattering work?

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



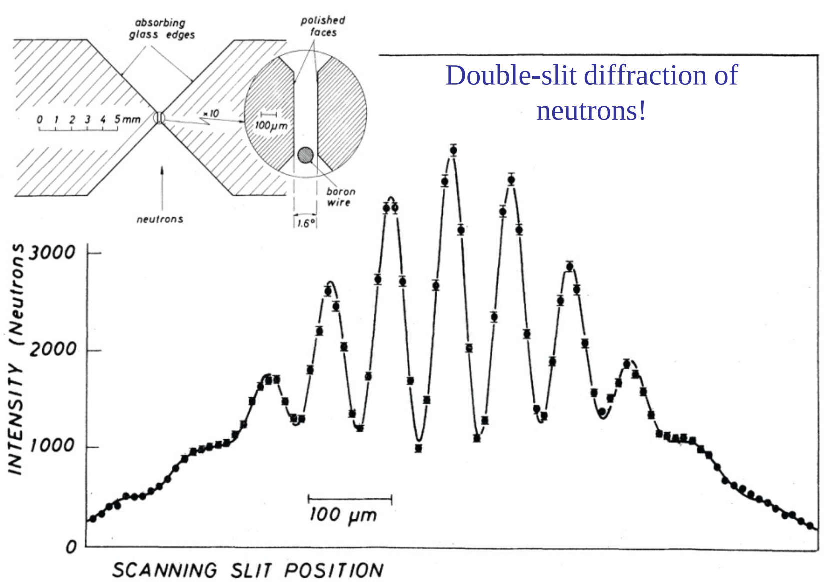
Nobel Prize 1929 for "for his discovery of the wave nature of electrons."

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**!

$E = mc^2 = (mc)c = pc = pf\lambda = hf$

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



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?

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

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

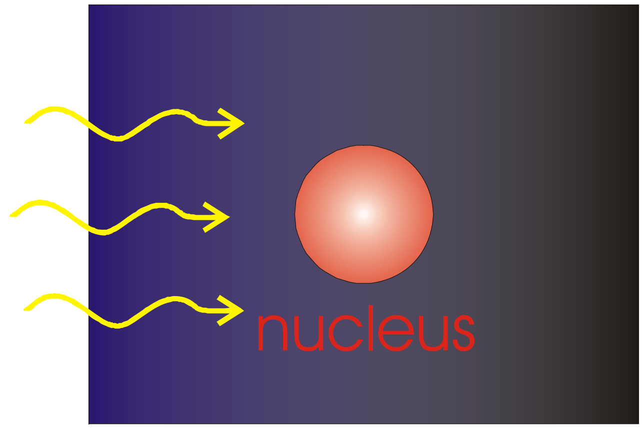
Maximum speed of a Ferrari: 105.5 ms^{-1}

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}: $\lambda = 1.5 \times 10^{-24}$ Å

Diffraction: single nucleus

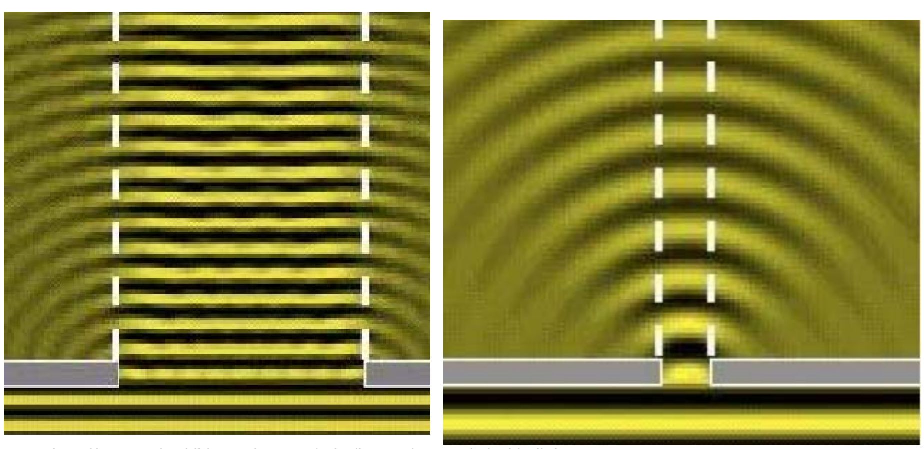


Single nucleus: analogy with diffraction of light:

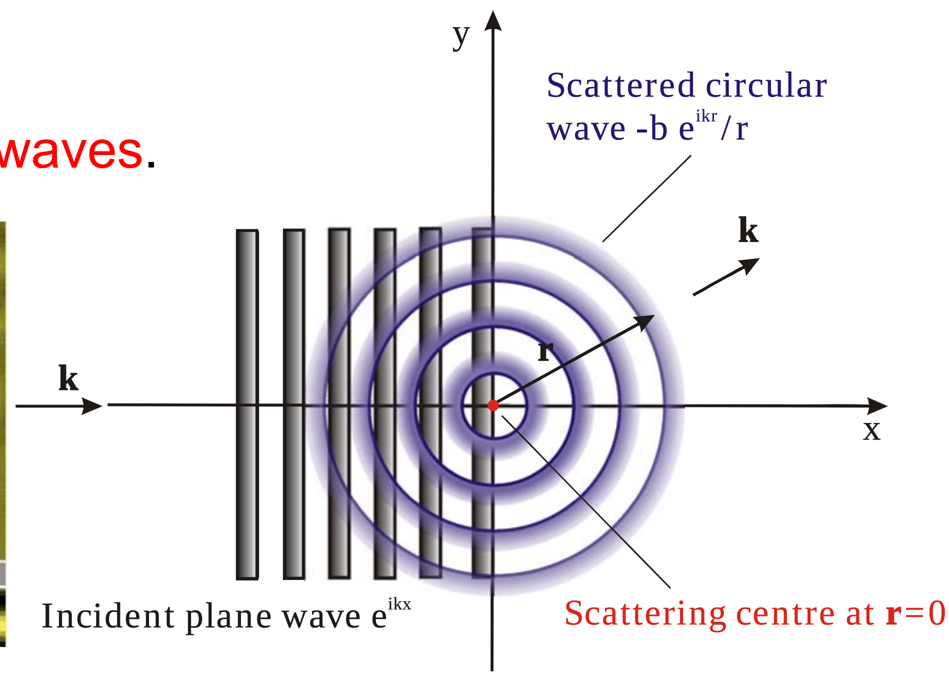
incident waves = plane waves
nucleus = ideal point scatterer

Nucleus scatters the incident neutron beam uniformly in all directions:

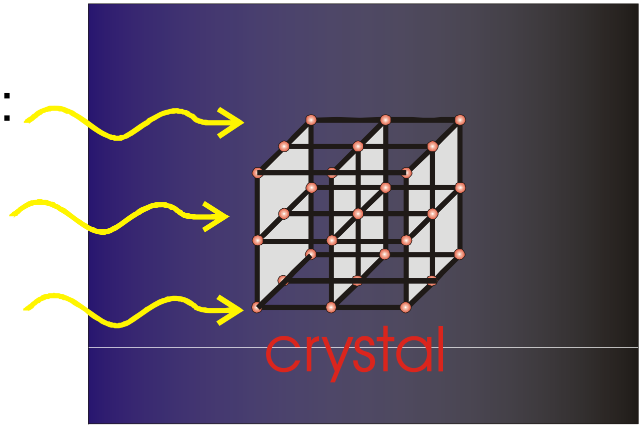
scattered waves = spherical isotropic waves.



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



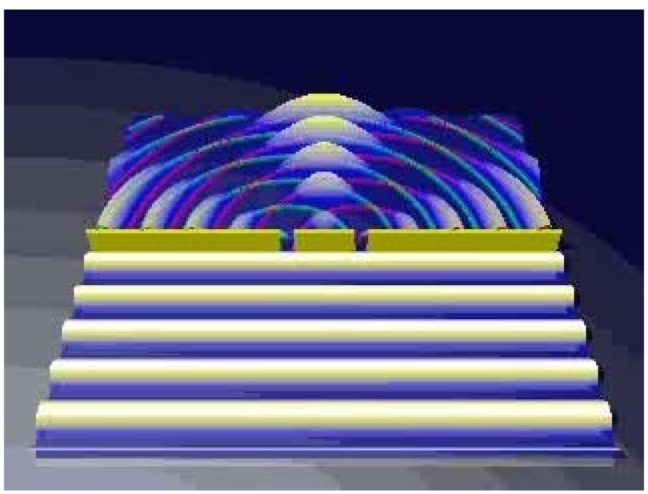
Diffraction: many nuclei in a crystal

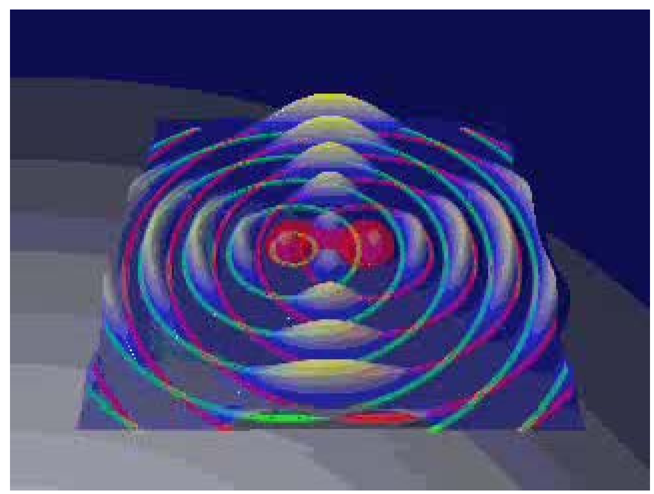


Many nuclei: analogy with diffraction of light again:

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.





Wave description

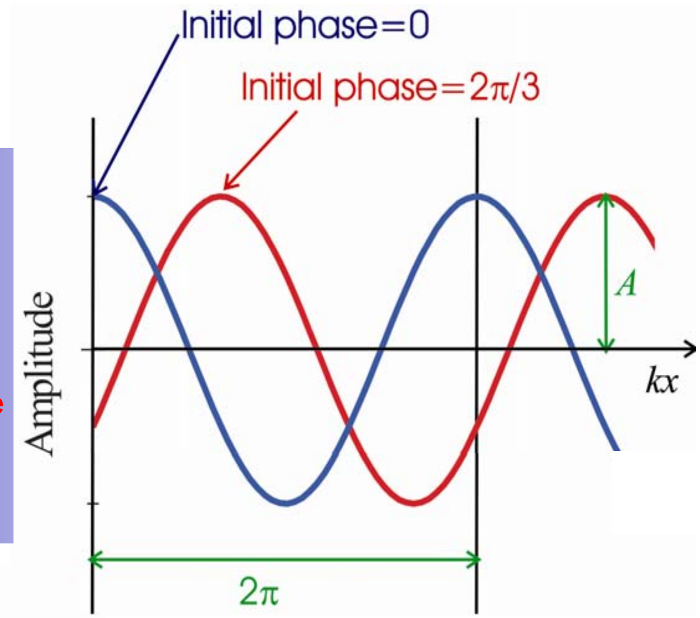
Diffraction due to interference between waves scattered elastically from nuclei in the crystal.

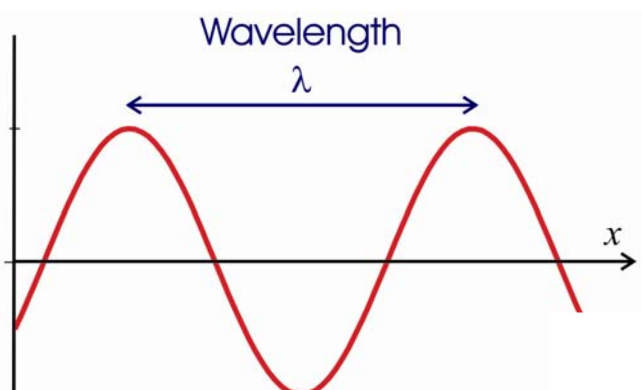
Intensity of a wave moving with a velocity v along x-direction, at any given position is:

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

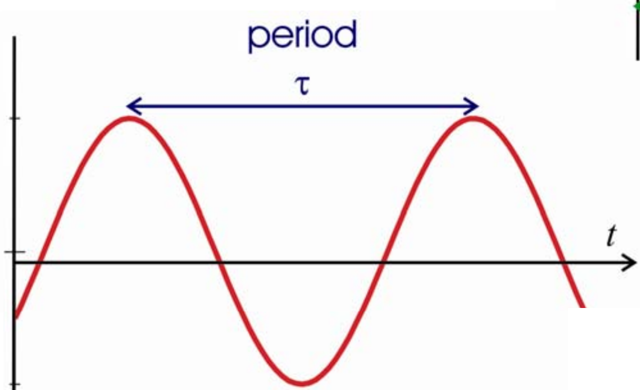
amplitude — k-vector — Angular freq. — Initial phase

$$k = \frac{2\pi}{\lambda} \qquad \omega = \frac{2\pi}{\tau}$$





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



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

Phase velocity:

$$v = \lambda / \tau$$

$$v = \lambda \nu$$

$$v = \omega / k$$

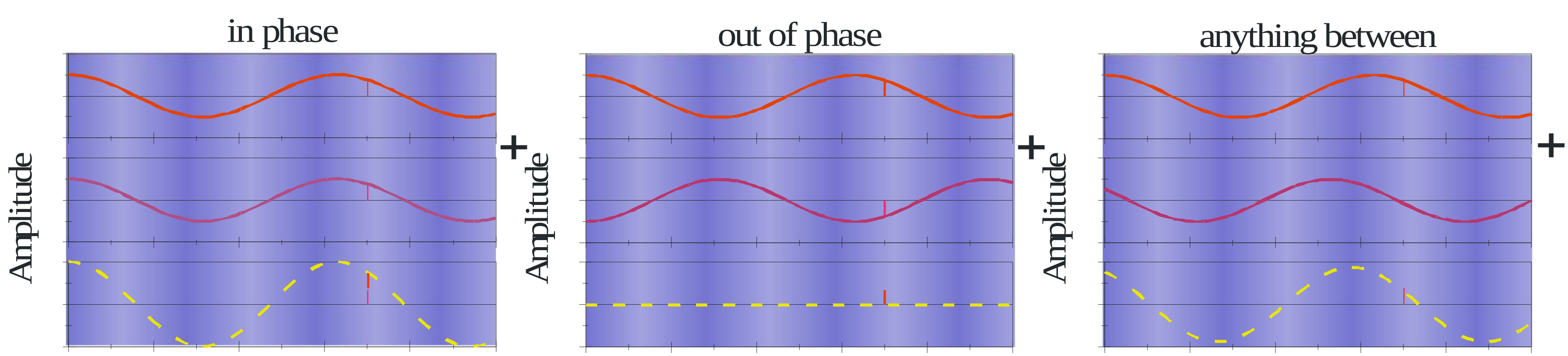
Addition of waves

Adding waves with the same wavelength but different initial phase:

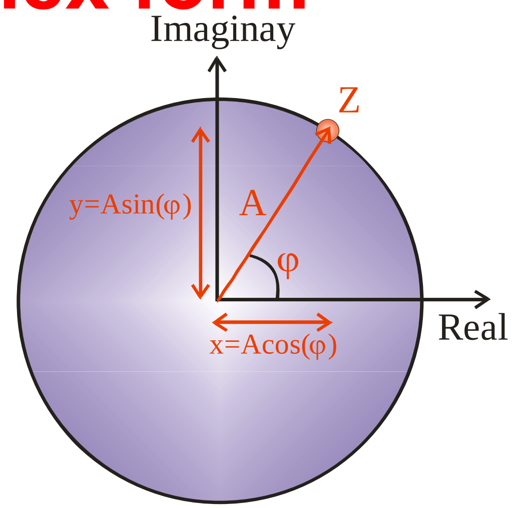
- **constructive**: if exactly in phase ($\Delta\phi = \lambda$), maximum possible amplitude.

- **destructive**: if exactly out of phase ($\Delta\phi = \lambda/2$), zero amplitude.

- **anything between:** if partially out of phase ($\Delta\phi$), anything between amplitude.



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:

$$Z = x + i\,y = A\cos(\varphi) + i\,A\sin(\varphi)$$

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

Can a plane **wave** can 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: $\tan(\varphi)=\mathrm{Im}\{Z\}/\mathrm{Re}\{Z\}$.

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!

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

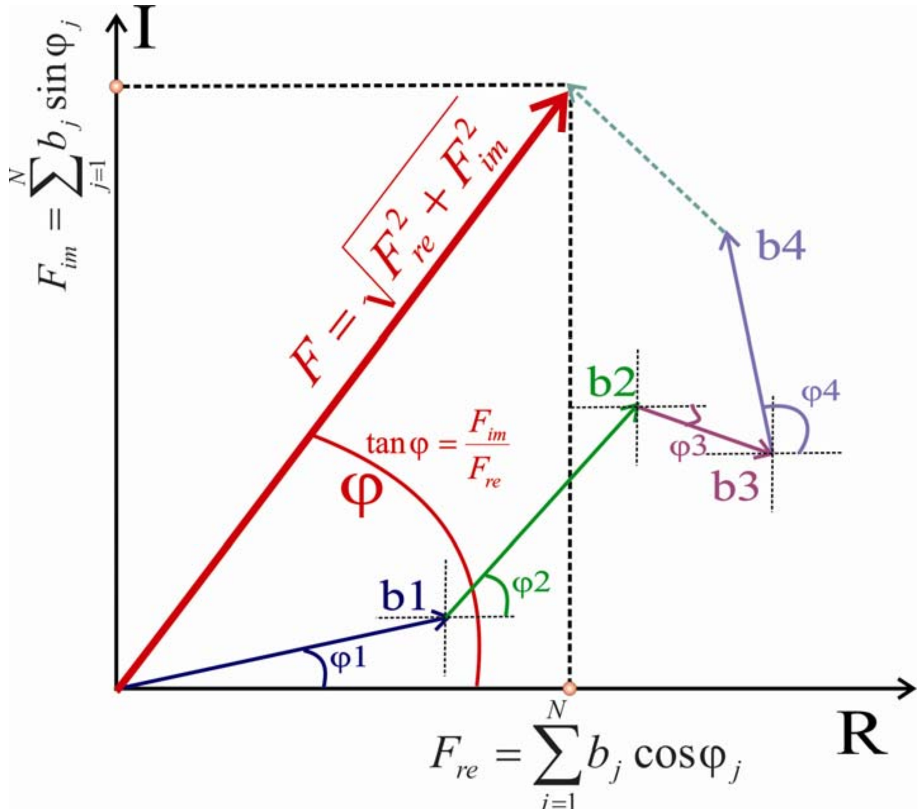
$$\underset{\sim}{F}_{tot}(x,t) = \underset{\sim}{F}_1\, e^{i(kx-\omega t)} + \underset{\sim}{F}_2\, e^{i(kx-\omega t)} + \ldots$$

$$= (\underset{\sim}{F}_1 + \underset{\sim}{F}_2 + \ldots)\, e^{i(kx-\omega t)}$$

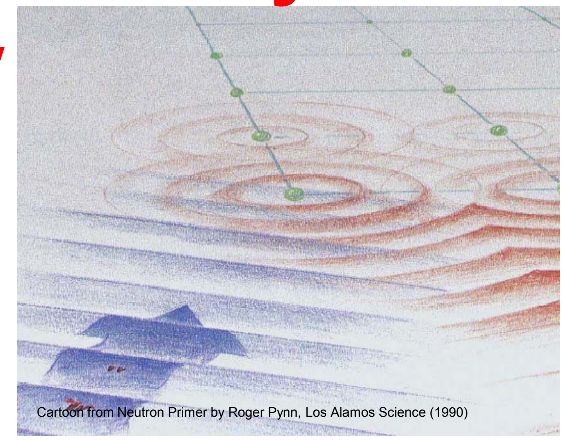
$$= (b_1 e^{i\varphi_1} + b_2 e^{i\varphi_2} + \ldots)\, e^{i(kx-\omega t)}$$

$$= \underset{\sim}{F}_{tot}\, e^{i(kx-\omega t)}$$

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



Diffraction from crystals: Bragg's law



- 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 → solve a variety of problems!

Diffraction from crystals: Bragg's law

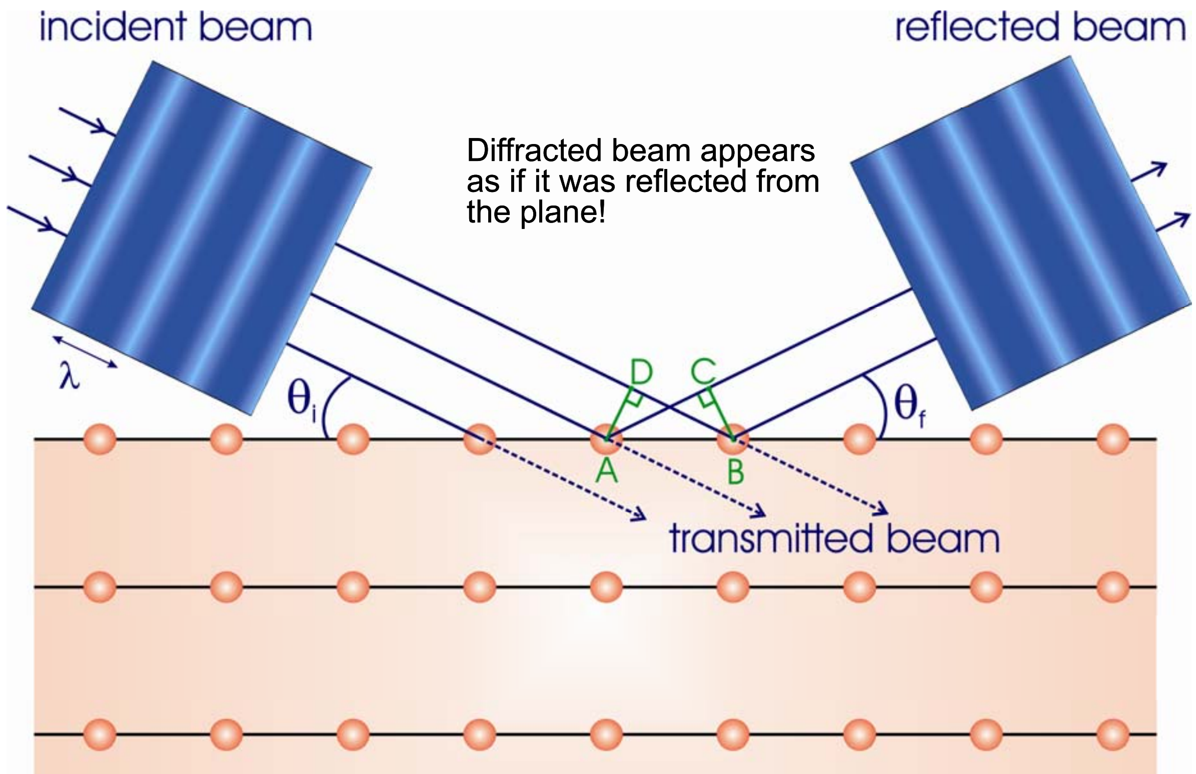
Diffraction from a single layer of atoms: Specular reflection.

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

$$\theta_i = \theta_f$$



Diffraction from crystals: Bragg's law

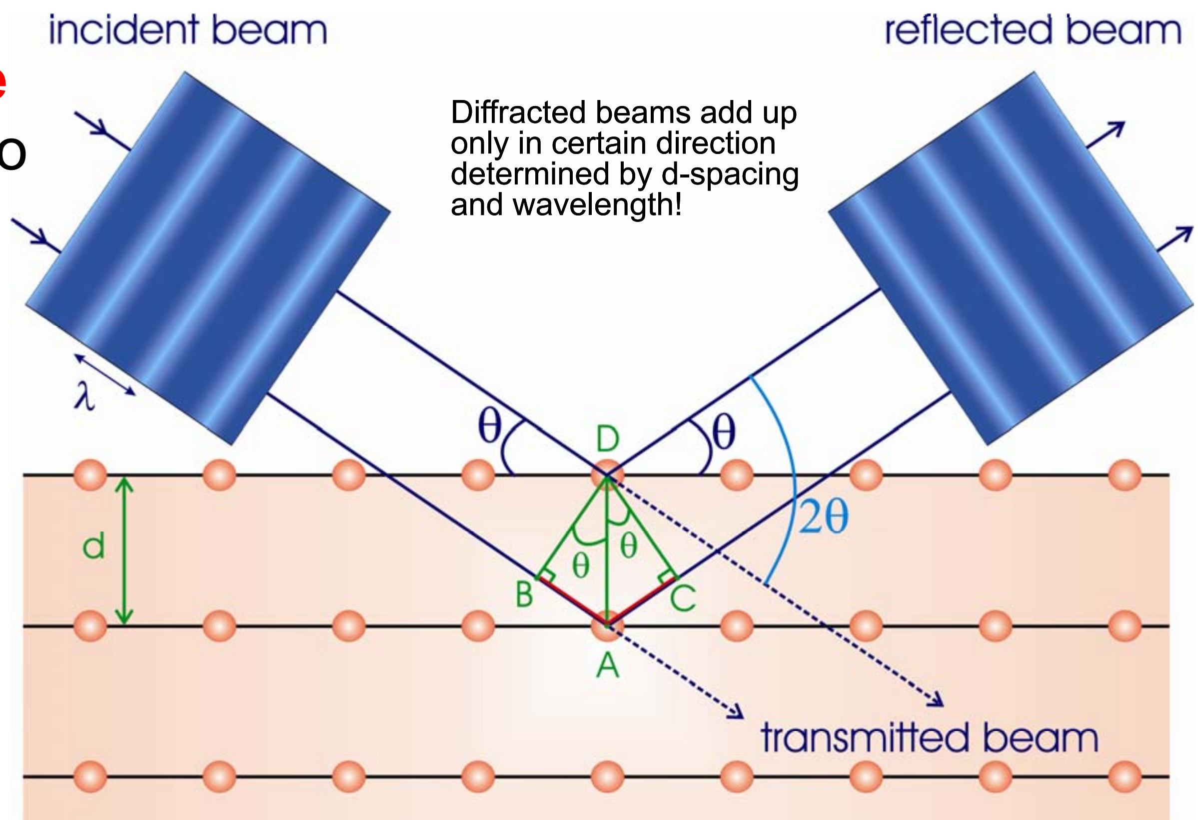
Diffraction: neutrons interact with nuclei → scattered in all directions by every nucleus they encounter. Scattered waves from different nuclei travel different distances → acquire different phase → interfere as they add up!

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

$$AB + AC = n\lambda$$

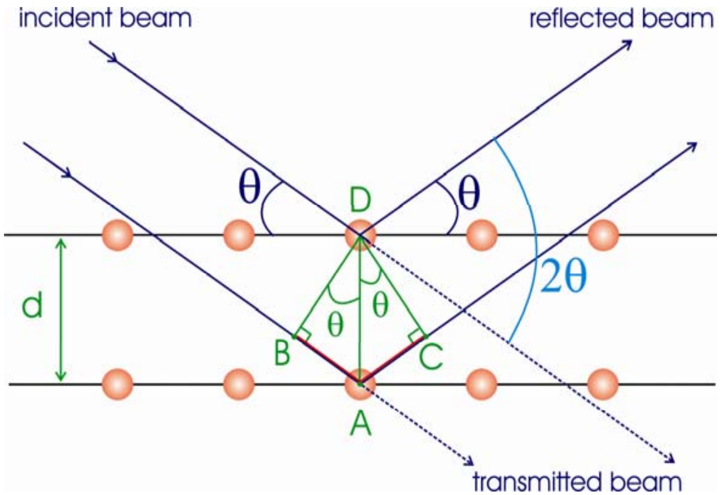
$$2d \sin\theta = n\lambda$$

Bragg's Law



More on Bragg's law

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



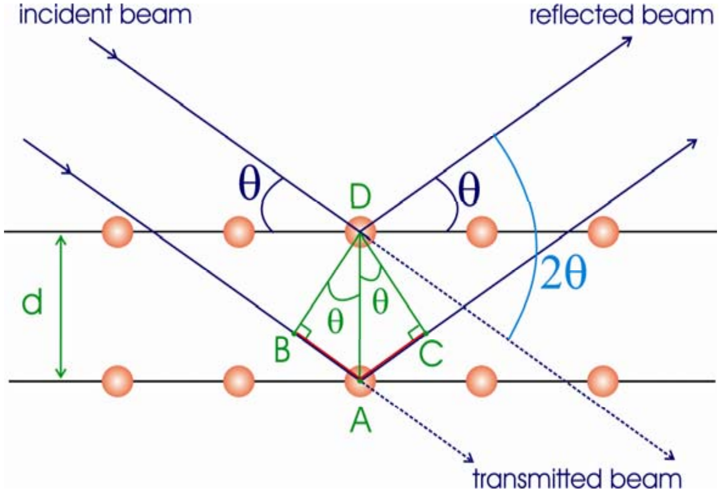
- Diffraction peaks observed only when successive planes scatter in phase (it is relative phase that matters): Coherent scattering from a single plane not sufficient.

- 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 $\lambda=2d_{max}$?

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: $d_{nh\,nk\,nl} = \frac{d_{hkl}}{n} \rightarrow 2d_{hkl} \sin\theta = \lambda$.
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).

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

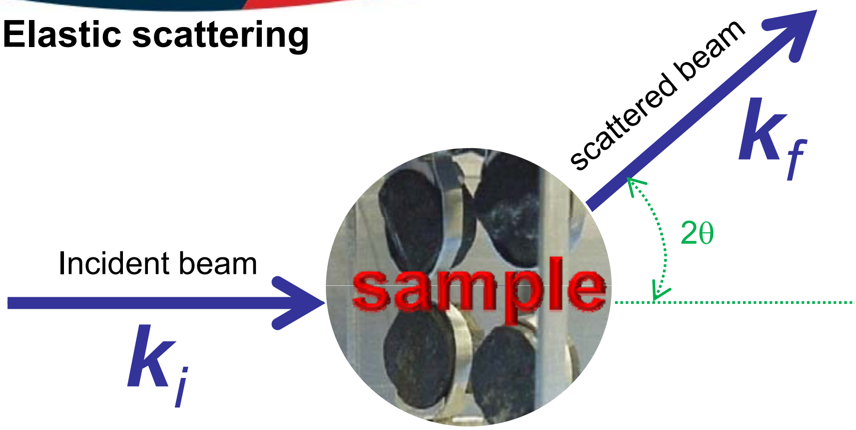
$$|\psi|^2 = \psi \times \psi^*$$

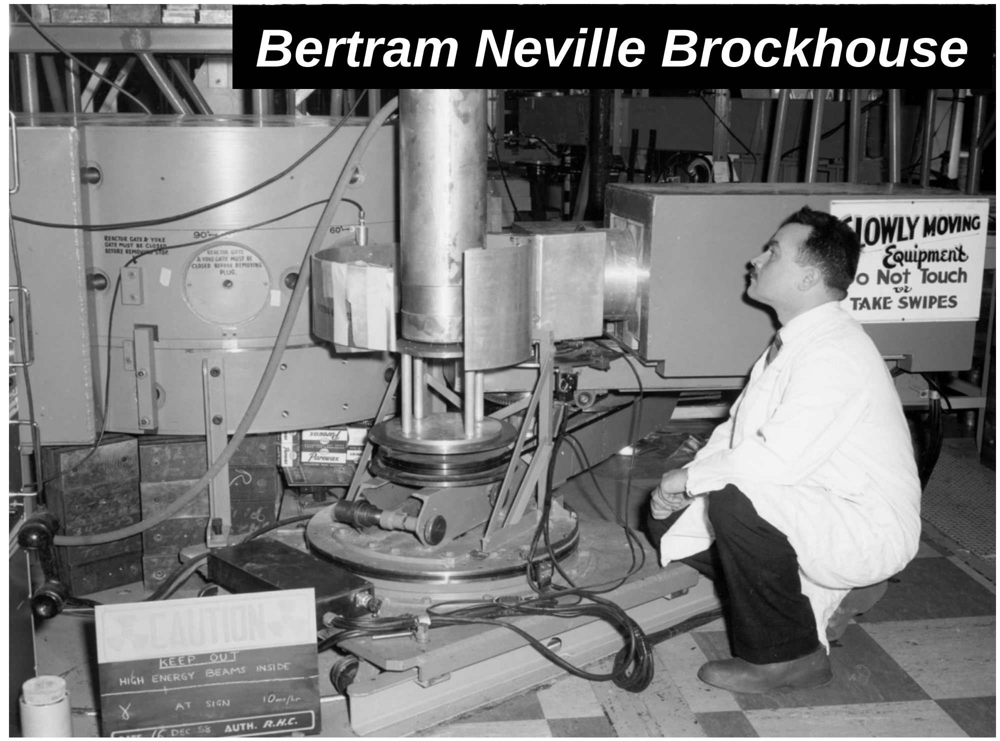
Neutron wavevector ***k***: a vector pointing along neutron's trajectory.

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

How is it related to experiment?

Elastic scattering





Scattering vector

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

Conservation of momentum

Momentum transfer= $\hbar \mathbf{Q}$ with $|\mathbf{Q}| = Q = 4\pi \sin\theta/\lambda$

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.

Scattering by a fixed single nucleus

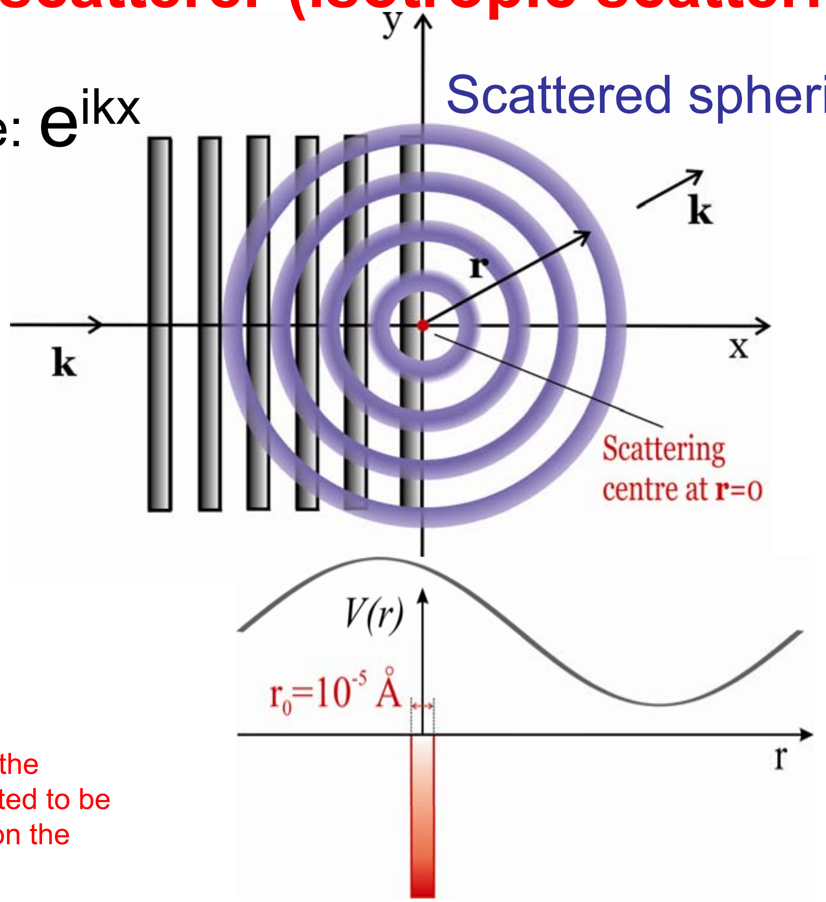
Neutrons interact with matter via nuclear force: very short range ~10^{-15} m, size of a nucleus ~100,000 times smaller than distance between centers!

Nucleus → **point scatterer (isotropic scattering)!**

Incident plane wave: e^{ikx}

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

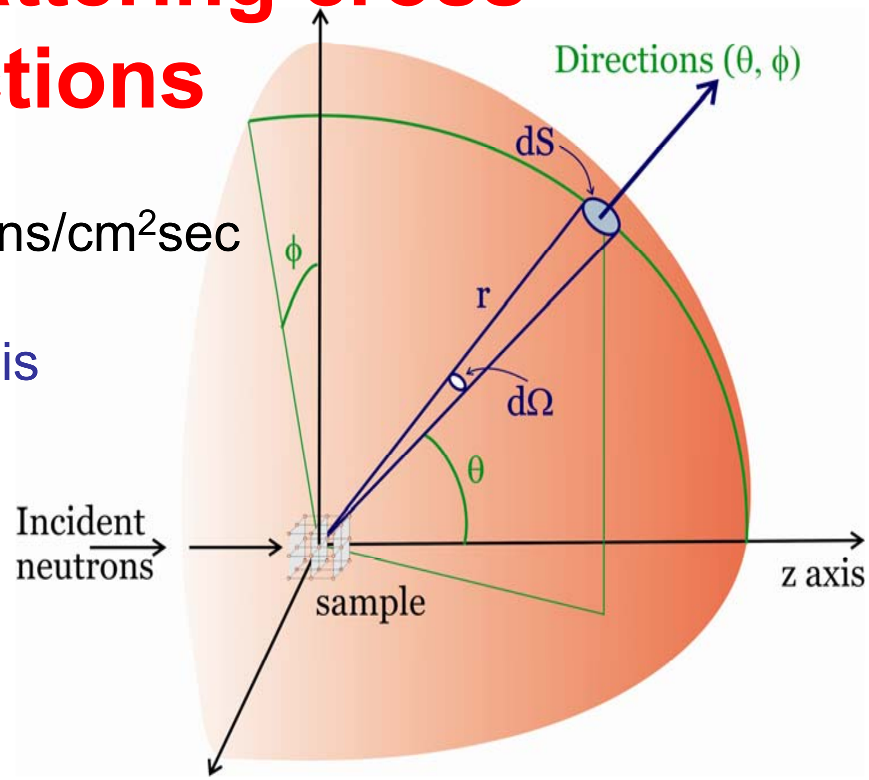
Squared modulus =1 anywhere, neutron is found with same probability at all positions!



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!

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:

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

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)

Cross-section for a fixed single nucleus

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

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

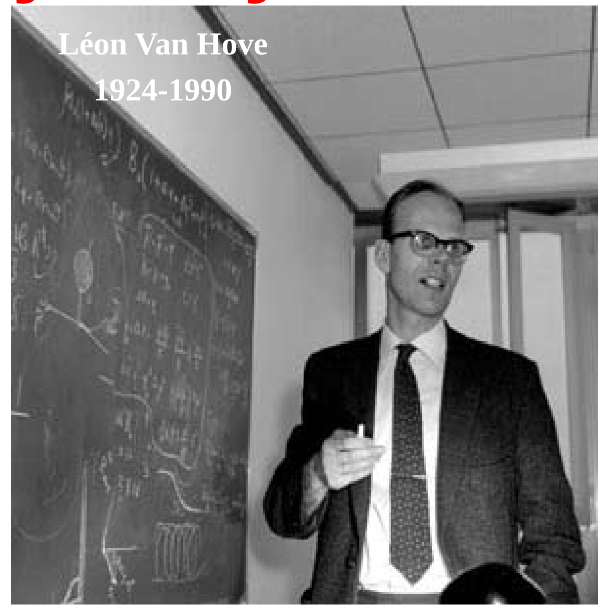
Number of scattered neutrons with a velocity v passing through area dS:

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

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

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

Scattering by many fixed nuclei



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

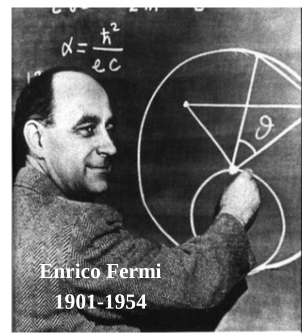
Pseudo-potential (Fermi): interaction between a neutron and a nucleus is replaced by a much weaker effective potential.

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

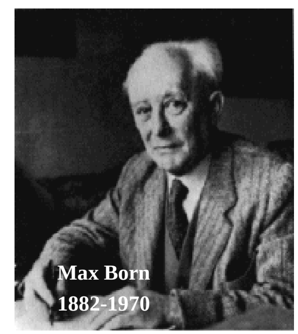
Scattering law (Van Hove): probability of a neutron wave $\mathbf{k}_i$ being scattered by V($\mathbf{r}$) into outgoing wave of $\mathbf{k}_f$ is:

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

Integration is over the volume of the sample.



Nobel Prize 1938 for "his work on induced radioactivity"



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

Scattering by many fixed nuclei

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

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

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

$$\frac{d\sigma}{d\Omega} = \left(\frac{m}{2\pi\hbar^2}\right)^2 \left|\int V(\mathbf{r}')e^{i\mathbf{r}'.(\mathbf{k}_i - \mathbf{k}_f)} d\mathbf{r}'\right|^2$$

$$= \left(\frac{m}{2\pi\hbar^2}\right)^2 \left|\int \sum_{\mathbf{j}} \mathrm{b}_{\mathbf{j}} \left(\frac{2\pi\hbar^2}{m}\right) \delta(\mathbf{r}' - \mathbf{R}_j) e^{i\mathbf{r}'.\mathbf{Q}} d\mathbf{r}'\right|^2$$

$$= \left|\sum_{\mathrm{j}} \mathrm{b}_{\mathrm{j}} e^{i\mathbf{R}_{\mathbf{j}}.\mathbf{Q}}\right|^2 = \sum_{\mathrm{j,k}} \mathrm{b}_{\mathrm{j}} \mathrm{b}_{\mathrm{k}} e^{-i(\mathbf{R}_k - \mathbf{R}_j).\mathbf{Q}}$$

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

$$\frac{d\sigma}{d\Omega} = \left|\sum_{\mathrm{j}} \mathrm{b}_{\mathrm{j}} e^{i\mathbf{R}_{\mathbf{j}}.\mathbf{Q}}\right|^2 = \sum_{\mathrm{j,k}} \mathrm{b}_{\mathrm{j}} \mathrm{b}_{\mathrm{k}} A_{jk} = \sum_{\mathrm{j,k}} \overline{\mathrm{b}}^2 A_{jk} + \sum_j \left(\overline{\mathrm{b}^2} - \overline{\mathrm{b}}^2\right) A_{jj}$$

coherent incoherent

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 $b_j = b_k$:

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

$$\mathrm{G}(\mathbf{r}) = \frac{1}{\mathrm{N}} \sum_{j,k} \delta(\mathbf{r} - (\mathbf{R}_j - \mathbf{R}_k))$$

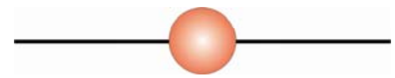
Fourier transform of pair correlation function G(**r**)

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.

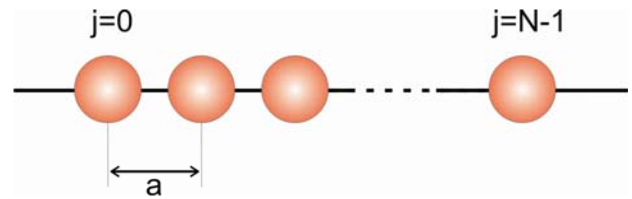
Evaluating the double sum

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

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



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

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

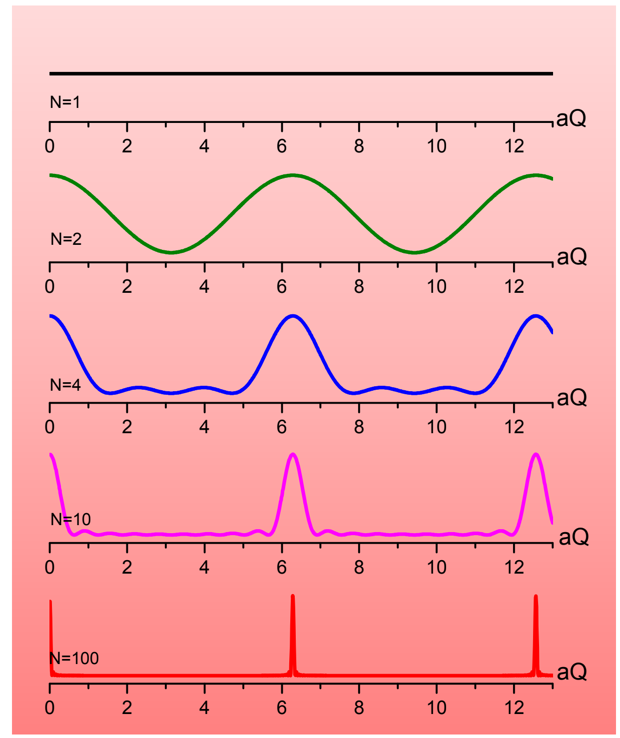
Reciprocal!

In 3D:

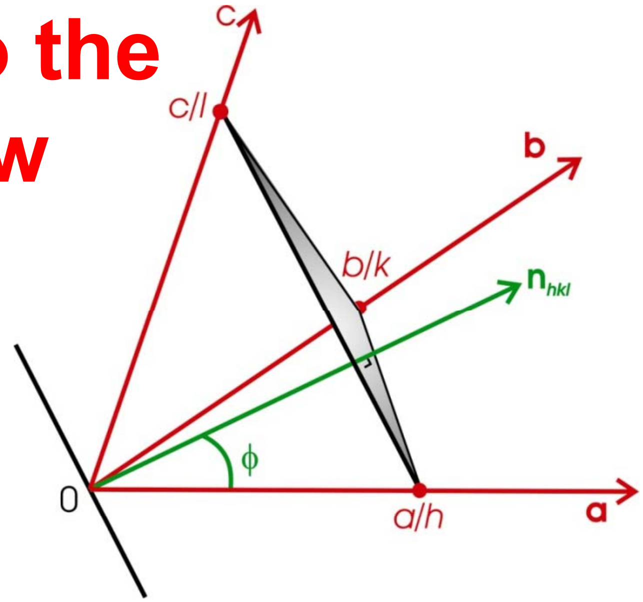
a.Q$_{\mathrm{Bragg}}$=2π*m*, b.Q$_{\mathrm{Bragg}}$=2π*n*, c.Q$_{\mathrm{Bragg}}$=2π*p*

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…



Relation to the Bragg's law



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

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

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

In 3D:

$\mathbf{a}.\mathbf{Q}_{Bragg}=2\pi m$, $\mathbf{b}.\mathbf{Q}_{Bragg}=2\pi n$, $\mathbf{c}.\mathbf{Q}_{Bragg}=2\pi p$

m, n, p: integer

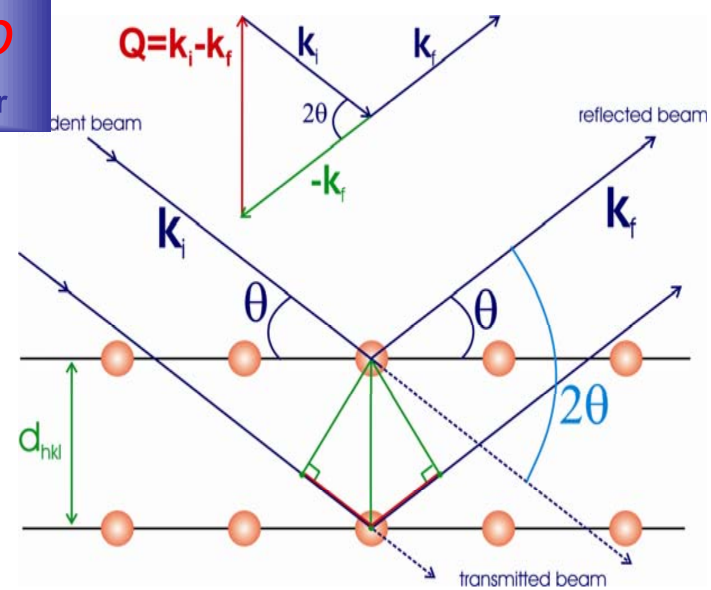
Laue condition

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

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

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

Scattering triangle



Many nuclei: Structure factor

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

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.

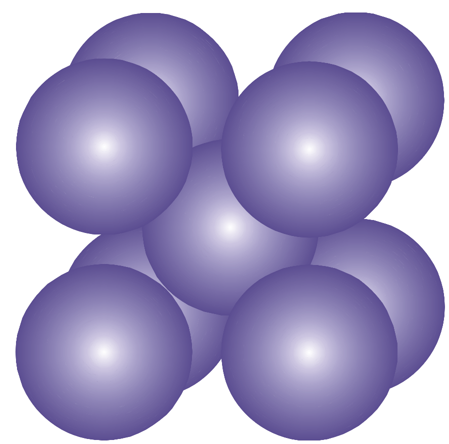
$$\mathrm{F}(\mathbf{Q}) = \sum_{\text{all nuclei}} \mathrm{b}_j e^{i\mathbf{R}_j.\mathbf{Q}} = \underbrace{\sum_{\text{lattice}} e^{i\mathbf{T}.\mathbf{G}_{\mathbf{hkl}}}}_{\text{N}} \; \underbrace{\sum_{\text{basis}} \mathrm{b}_j e^{i\mathbf{r}_j.\mathbf{G}_{\mathbf{hkl}}}}_{\text{Structure factor}}$$

Structure Factor:

$$\mathrm{F}_{hkl} = \sum_{basis} \mathrm{b}_j e^{i2\pi(hu_j + kv_j + lw_j)}$$

Complex number

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



Reciprocal Space

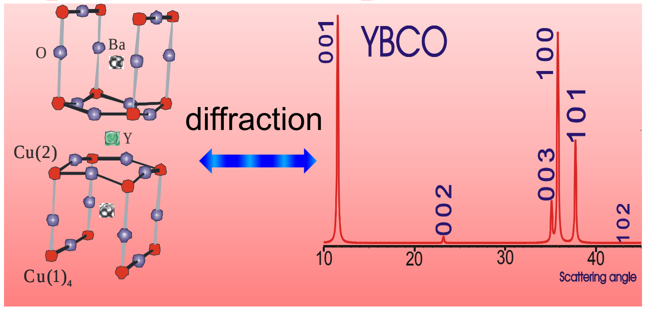
Reciprocal features so far?

- Inverse relation between d and θ.
- Miller indices: reciprocal (or inverse) of unit cell intercepts.
- Intensity is proportional to Fourier transform of pair correlation function!

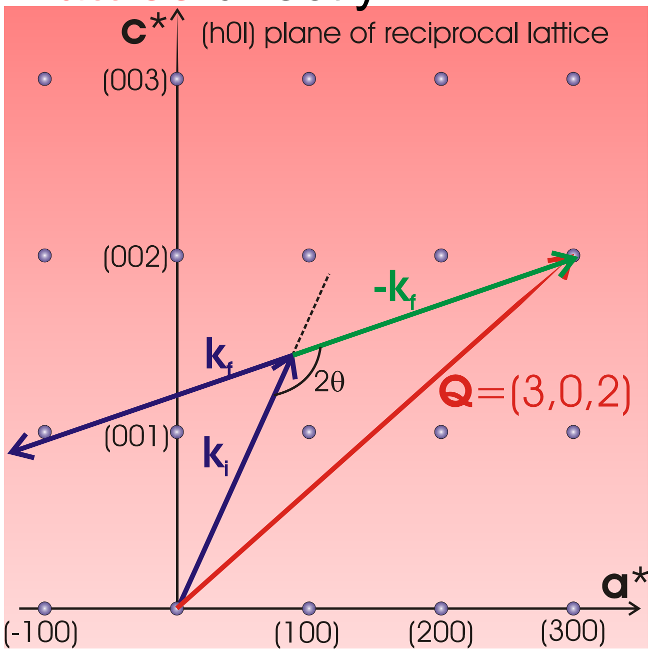
$$2d_{hkl}\sin\theta = \lambda$$

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

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



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



reciprocal lattice:

Reciprocal lattice vector: $G_{hkl} = ha^* + kb^* + lc^*$

Compare with real lattice: $T_{uvw} = ua + vb + wc$

Reciprocal unit cell vectors:

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

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

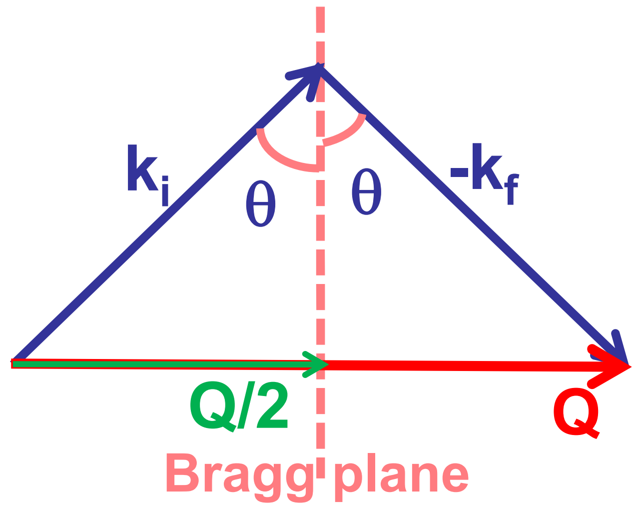
Brillouin Zones

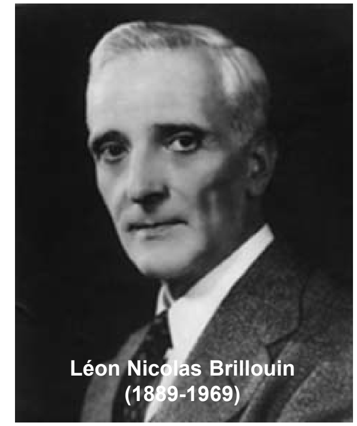
Bragg condition in reciprocal space for elastic $|\mathbf{k}_i| = |\mathbf{k}_f|$:

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

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

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



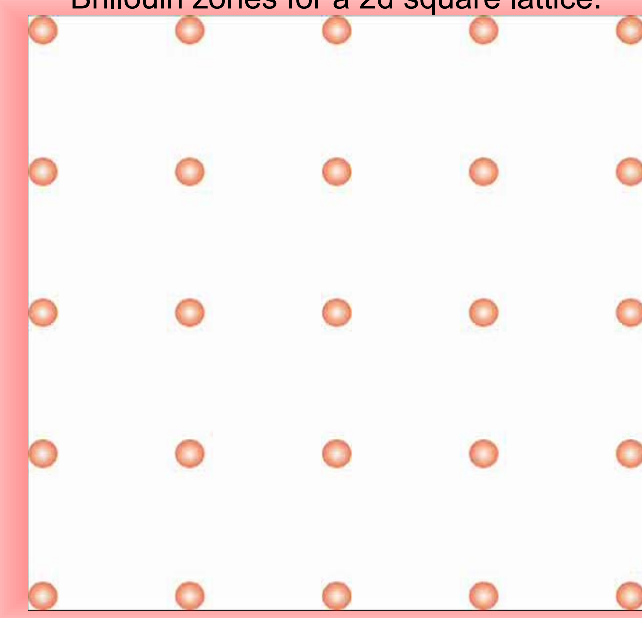


Brillouin zones are widely used in condensed matter physics: theory of electron bands and other types of excitations.

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:



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