

Diffraction From Powder (Polycrystalline) Samples and Structure Determination

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Neutron Scattering's Moment in the Limelight

The Nobel Prize in Physics 1994



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



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

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

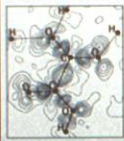
The pattern also shows how atomic dipoles are oriented in magnetic materials, since neutrons are affected by magnetic forces. Shull also made use of this phenomenon in his neutron diffraction technique.



In early (1950) neutron diffractometer with flexible wavelength control here used by E.O. Wollan and C.G. Shull (standing) at Oak Ridge National Laboratory.

Neutrons see more than X-rays

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



Let a neutron diffraction map (showing the positions of the nuclei) live as a 3-D diffraction map (giving the distribution of the electrons). It is then clear that the electron density is shifted in relation to the positions of the atomic nuclei. Since a chemical bond involves a shift in electron position, a direct picture of the chemical bond is obtained in this way.

Neutrons reveal inner stresses

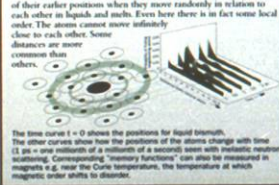
A hole has been punched in an important metal aircraft part. Does the part match up? Neutron diffraction can show how much the distance between the atoms has changed and hence the internal forces remaining around the hole after it has been punched!



The curves show local expansion forces (positive) and compression forces (negative) in different directions (red, green and blue) in the straight part (dash-dot-dot part) (dash-dot-dot part).

Neutrons show what atoms remember

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



The time curve $t = 0$ shows the positions for liquid bromine. The other curves show how the positions of the atoms change with time (1, 20, or one millisecond of a second) seen with neutron spin scattering. Corresponding "memory functions" can also be measured in magnets, e.g. near the Curie temperature, the temperature at which magnetic order shifts to disorder.

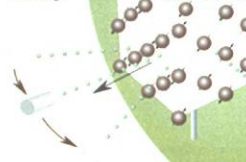
Neutrons behave as particles and as waves

Neutrons reveal structure and dynamics

Neutrons show where atoms are

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

Atoms in a crystalline sample



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

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

Research reactor

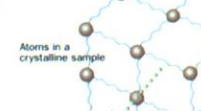


3-axis spectrometer

Neutrons show what atoms do

3-axis spectrometer with rotatable crystals and rotatable sample

Atoms in a crystalline sample



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

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

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

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

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

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



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

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

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

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



Lecture Outline -- References

- ◆ General Concepts
- ◆ Direct Lattice, Reciprocal Lattice, Lattice Types
- ◆ Diffraction Conditions (Bragg Law, Ewald Diagram)
- ◆ Polycrystals vs Single Crystals
- ◆ Scattering Cross-sections, amplitudes and form factors
- ◆ References:
 - *Neutron Diffraction*, G.E. Bacon, 5th edition, Oxford Press, 1975
 - *Theory of Neutron Scattering From Condensed Matter*, S.W. Lovesey, Oxford Press 1984
 - *Introduction to the Theory of Neutron Scattering*, G.L. Squires, Dover, 1996.
 - *Solid State Physics*, N.W. Ashcroft, N.D. Mermin, Holt, Rinehart & Winston, 1976

General Properties of the Neutron

- ◆ The kinetic energy of a 1.8 Å neutron is equivalent to $T = 293\text{K}$ (warm coffee!), so it is called a thermal neutron.
- ◆ The relationships between wavelength (Å) and the energy (meV), and the speed (m/s, mi/hr) of the neutron are:

$$E = 81.89 / \lambda^2 \quad \text{and} \quad v = 3960 / \lambda$$

e.g. the 1.8 Å neutron has $E = 25.3 \text{ meV}$ and $v = 2200 \text{ m/s} = 4900 \text{ mi/hr}$

- ◆ The wavelength is of the same order as the atomic separation so interference occurs between waves scattered by neighboring atoms (diffraction).
- ◆ Also, the energy is of same order as that of lattice vibrations (phonons) or magnetic excitations (magnons) and thus creation or annihilation of a lattice wave produces a measurable shift in neutron energy (inelastic scattering).

COMPARATIVE PROPERTIES OF X-RAY AND NEUTRON SCATTERING

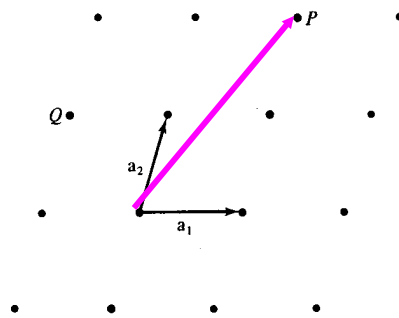
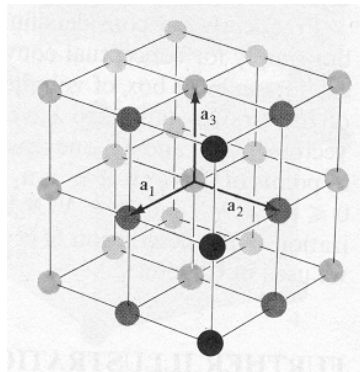
Property	X-Rays	Neutrons
Wavelength	Characteristic line spectra such as Cu K_{α} $\lambda = 1.54 \text{ \AA}$	Continuous wavelength band, or single $\lambda = 1.1 \pm 0.05 \text{ \AA}$ separated out from Maxwell spectrum by crystal monochromator or chopper
Energy for $\lambda = 1 \text{ \AA}$	10^{18} h	10^{13} h (same order as energy of elementary excitations)
Nature of scattering by atoms	Electronic Form factor dependence on $[\sin\theta]/\lambda$ Linear increase of scattering amplitude with atomic number, calculable from known electronic configurations	Nuclear, Isotropic, no angular dependent factor Irregular variation with atomic number. Dependent on nuclear structure and only determined empirically by experiment
Magnetic Scattering	Very weak additional scattering ($\approx 10^{-5}$)	Additional scattering by atoms with magnetic moments (same magnitude as nuclear scattering) Amplitude of scattering falls off with increasing $[\sin \theta]/\lambda$
Absorption coefficient	Very large, true absorption much larger than scattering $\mu_{\text{abs}} \approx 10^2 - 10^3$ increases with atomic number	Absorption usually very small (exceptions Gd, Cd, B ...) and less than scattering $\mu_{\text{abs}} \approx 10^{-1}$
Method of Detection	Solid State Detector, Image Plate	Proportional ^3He counter

Real Space Lattice

Direct Space Vectors, Unit Cells

- ◆ Bravais Lattice -- Lattice of Atoms in Crystal Cell

- Basis vectors $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$

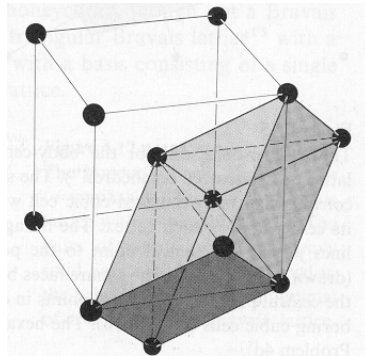


- Vector to $\mathbf{P} = \mathbf{a}_1 + 2 \mathbf{a}_2$ (2-D)
Linear Comb. Of Basis Vectors
 - General Vector (3-D)

$$\mathbf{R} = n_1 \mathbf{a}_1 + n_2 \mathbf{a}_2 + n_3 \mathbf{a}_3$$

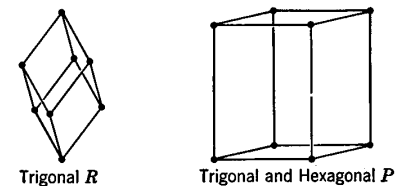
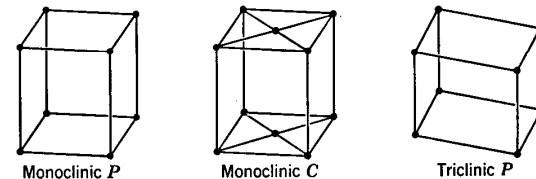
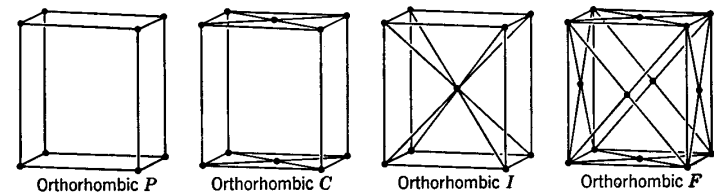
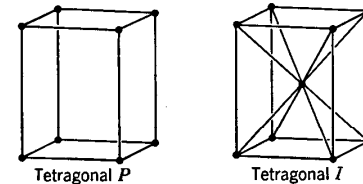
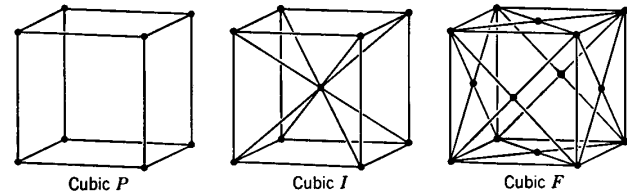
Cartoon *Neutron Man* from the LANSCE Neutron Scattering Primer

- ◆ *Primitive* Unit Cell contains only one atom
- ◆ (*Full*) Unit Cell may contain multiple primitive unit cells -- useful to describe full atomic symmetry (e.g., bcc has 2)



Types of 3-d Bravais Lattices

- ◆ 14 types of Bravais lattices in 7 classes
- ◆ Restricted Translations, Rotations, Mirror Planes, etc. are all allowed symmetry operations on lattice and generate 32 crystal classes and in turn 230 space groups



System	Number of lattices	Restrictions on conventional cell axes and angles
Triclinic	1	$a_1 \neq a_2 \neq a_3$ $\alpha \neq \beta \neq \gamma$
Monoclinic	2	$a_1 \neq a_2 \neq a_3$ $\alpha = \gamma = 90^\circ \neq \beta$
Orthorhombic	4	$a_1 \neq a_2 \neq a_3$ $\alpha = \beta = \gamma = 90^\circ$
Tetragonal	2	$a_1 = a_2 \neq a_3$ $\alpha = \beta = \gamma = 90^\circ$
Cubic	3	$a_1 = a_2 = a_3$ $\alpha = \beta = \gamma = 90^\circ$
Trigonal	1	$a_1 = a_2 = a_3$ $\alpha = \beta = \gamma < 120^\circ, \neq 90^\circ$
Hexagonal	1	$a_1 = a_2 \neq a_3$ $\alpha = \beta = 90^\circ$ $\gamma = 120^\circ$

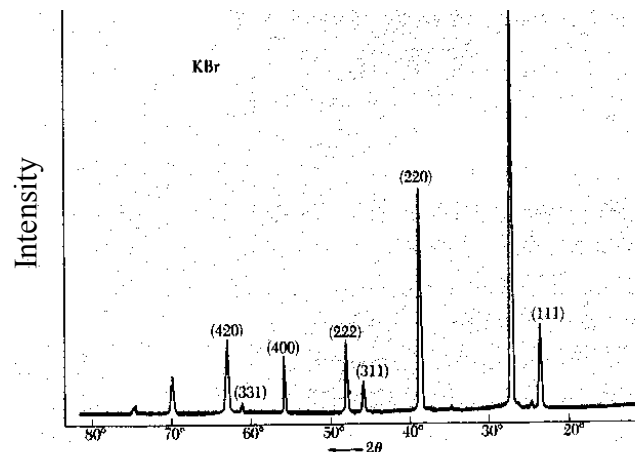
Golden Rule of Neutron Scattering

- ◆ We don't take pictures of atoms!

Atoms in fcc crystal



- ◆ Job preservation for neutron scatterers – we live in *reciprocal space*



Reciprocal Lattice (*also* Bravais)

- ◆ Vector \mathbf{R} of real space lattice $\mathbf{R} = n_1 \mathbf{a}_1 + n_2 \mathbf{a}_2 + n_3 \mathbf{a}_3$
- ◆ Incident plane wave $e^{i\mathbf{k}\cdot\mathbf{r}}$ [$|\mathbf{k}|=2\pi/\lambda$] will have periodicity of Bravais lattice for specific $\mathbf{k} = \mathbf{K}$:

$$e^{i\mathbf{K}\cdot(\mathbf{r} + \mathbf{R})} = e^{i\mathbf{K}\cdot\mathbf{r}} \quad \text{if } e^{i\mathbf{K}\cdot\mathbf{R}} = 1 \quad \text{or } \mathbf{K}\cdot\mathbf{R} = 2\pi m$$

- ◆ Defines \mathbf{K} = reciprocal lattice vector (in *fake* scattering space)
 $\mathbf{K} = k_1 \mathbf{b}_1 + k_2 \mathbf{b}_2 + k_3 \mathbf{b}_3$ in terms of reciprocal lattice basis vectors \mathbf{b}_i
 $k_i = \text{integer}$ $\mathbf{b}_i = \text{defined as:}$

$$\vec{b}_1 = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{V}; \vec{b}_2 = 2\pi \frac{\vec{a}_3 \times \vec{a}_1}{V}; \vec{b}_3 = 2\pi \frac{\vec{a}_1 \times \vec{a}_2}{V}$$

$$\text{ex: } \vec{b}_1 \cdot \vec{a}_2 = 2\pi \frac{\vec{a}_2 \times \vec{a}_3 \cdot \vec{a}_2}{V} \equiv 0$$

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

$$\text{but } \vec{b}_2 \cdot \vec{a}_2 = 2\pi \frac{\vec{a}_3 \times \vec{a}_1 \cdot \vec{a}_2}{V} \equiv 2\pi$$

Note: $\mathbf{b}_i \cdot \mathbf{a}_j = 2\pi \delta_{ij}$ so

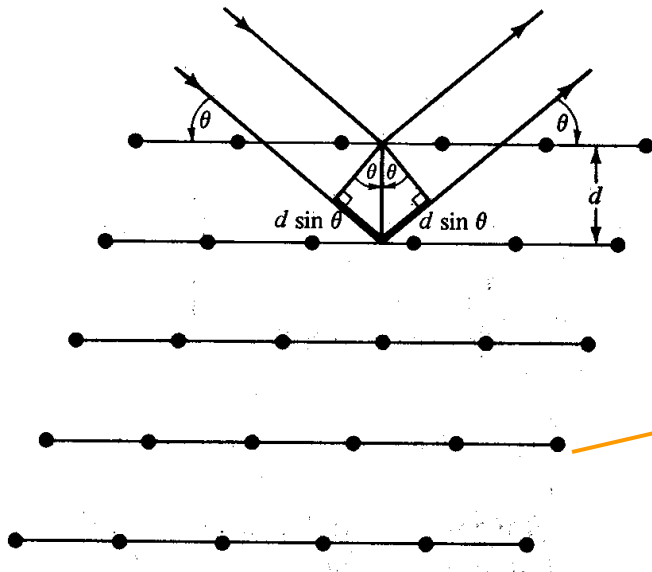
$\mathbf{K} \cdot \mathbf{R}$ satisfies periodicity (if k_i and n_i are integers)

- ◆ Reciprocal lattice of simple cubic cell is simple cubic cell of sides $2\pi/a$
- ◆ Reciprocal lattice of fcc cell is bcc cell of sides $4\pi/a$

Diffraction from a Crystal

Bragg Law, Laue formalism

- ◆ Incident x-rays or neutrons scatter from crystal planes



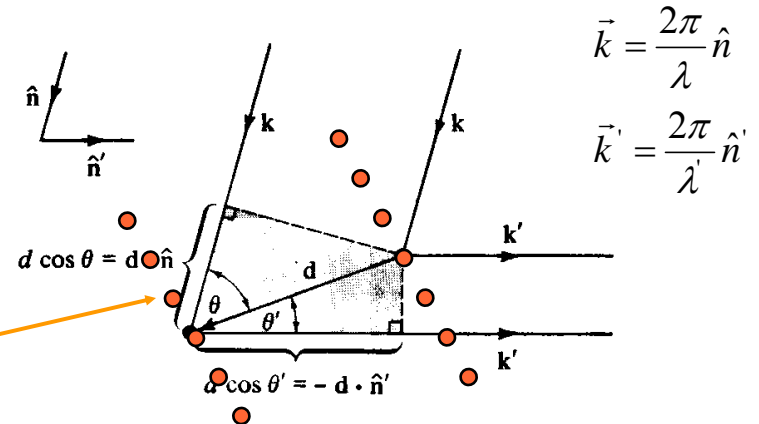
constructive interference

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

[Bragg Law]

- ◆ More generally

- incident wave of wavevector $\mathbf{k} = 2\pi/\lambda$
- scattered wave $\mathbf{k}' = 2\pi/\lambda'$



$$\vec{k} = \frac{2\pi}{\lambda} \hat{n}$$

$$\vec{k}' = \frac{2\pi}{\lambda'} \hat{n}'$$

- path difference:

$$d \cos\theta + d \cos\theta' = \mathbf{d} \cdot (\mathbf{n} - \mathbf{n}') = m \lambda$$

$$\text{or } \mathbf{d} \cdot (\mathbf{k} - \mathbf{k}') = 2\pi m$$

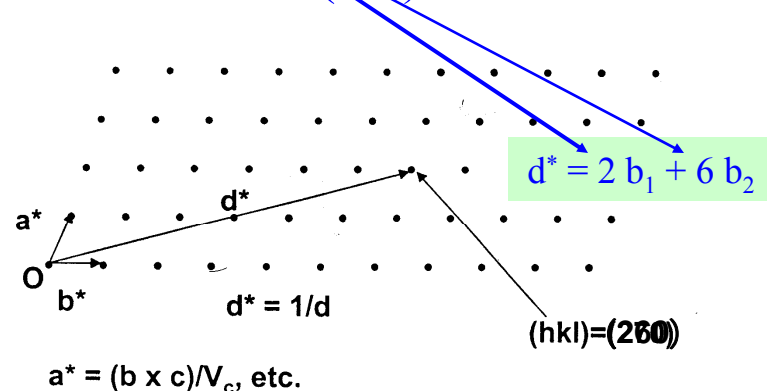
$$\text{or } \mathbf{R} \cdot \mathbf{K} = 2\pi m \quad [\text{Laue diffraction}]$$

$$\text{where Scat. Vec. } \mathbf{K} \text{ (or } \mathbf{Q}) = \mathbf{k} - \mathbf{k}' \quad 10$$

Crystal Diffraction, cont'd.

Diffraction conditions, Miller indices

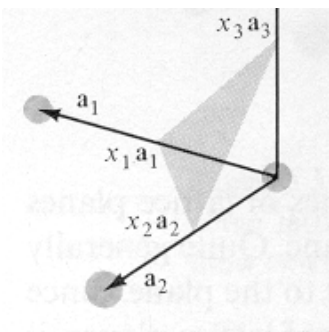
- ◆ Laue condition $\mathbf{R} \cdot \mathbf{K} = 2 \pi m$
or $e^{i\mathbf{K} \cdot \mathbf{R}} = 1$ for m integer
- ◆ Above is exactly the same as the definition of the reciprocal lattice
- ◆ Thus Laue diffraction condition satisfied if \mathbf{K} = recip. lat. vec.
- ◆ $\mathbf{K} = h \mathbf{b}_1 + k \mathbf{b}_2 + l \mathbf{b}_3$ -- defines Miller indices (hkl) of reflection



Note: $\mathbf{a}^*, \mathbf{b}^* \leftrightarrow \mathbf{b}_1, \mathbf{b}_2$

- ◆ Miller indices for a reflection have an analog in direct space
 - The direct space plane with Miller indices (hkl) is perpendicular to the reciprocal lattice vector

$$\mathbf{K} = h \mathbf{b}_1 + k \mathbf{b}_2 + l \mathbf{b}_3$$



$$h:k:l = \frac{1}{x_1} : \frac{1}{x_2} : \frac{1}{x_3}$$

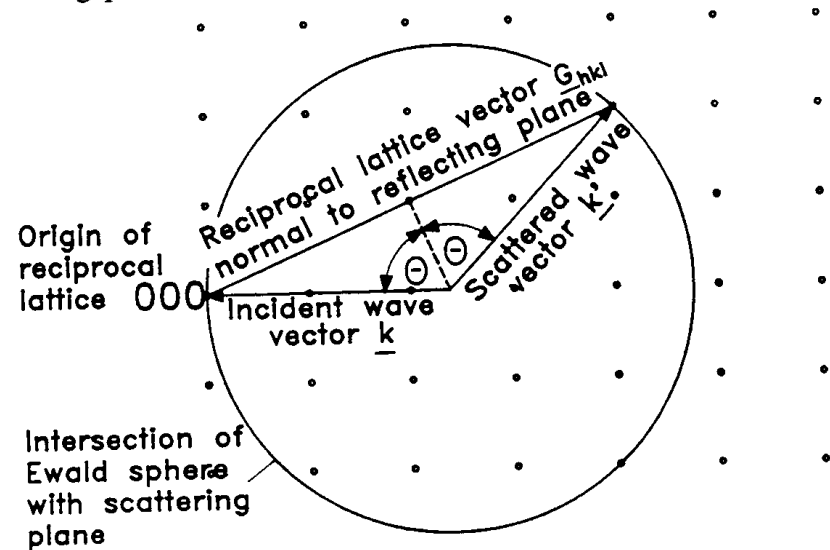
- Miller indices can have no common factors (shortest \mathbf{K})

Crystal Diffraction, cont'd.

Ewald Diagram

◆ Ewald Construction

- Sphere of radius $|\mathbf{k}|$ in reciprocal space
- Draw intersection of sphere with scattering plane
- Bragg condition satisfied if scattering vector $\mathbf{K} = \mathbf{k} - \mathbf{k}'$ is a Recip. Lat. Vector (i.e. Ewald sphere intersects recip. lat. Point)
- θ = angle of \mathbf{k} wrt crystal plane. 2θ = total deviation of x-ray (neutron) beam \equiv scattering angle

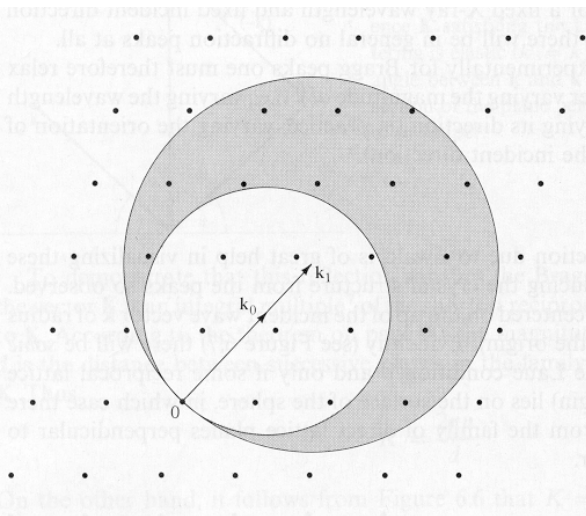


- ◆ Note: (100) (200) ... all refer to same crystal plane spacing (arise from higher order interference condition) [i.e. $2d\sin\theta = \underline{\mathbf{n}}\lambda$]
- ◆ Some (hkl) may not appear due to symmetry restrictions (space group)

Ewald Construction

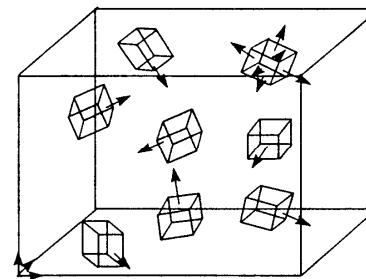
White Beam Diffraction, Polycrystals

- ◆ White Beam (e.g. LANSCE or IPNS) -- range of $k_0 < \mathbf{k} < k_0 + k_1$ simultaneously available



- ◆ Gray region spanned by available range of \mathbf{k}
- ◆ Large number of reflections accumulated simultaneously

- ◆ Previous discussion assumed scattering from ordered discrete atomic planes -- a single crystal
- ◆ Polycrystal (powder) - jumble of single crystals



All orientations of crystallites possible

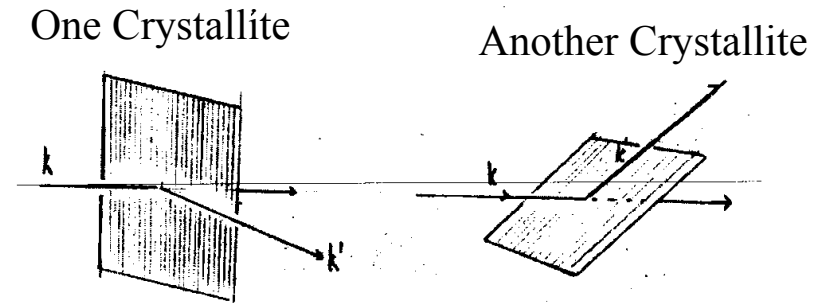
Sample: 1cc powder of $10\mu\text{m}$ crystallites - 10^9 particles
if $1\mu\text{m}$ crystallites - 10^{12} particles

- ◆ Several crystallites generally oriented to produce reflection for all allowed \mathbf{k} .

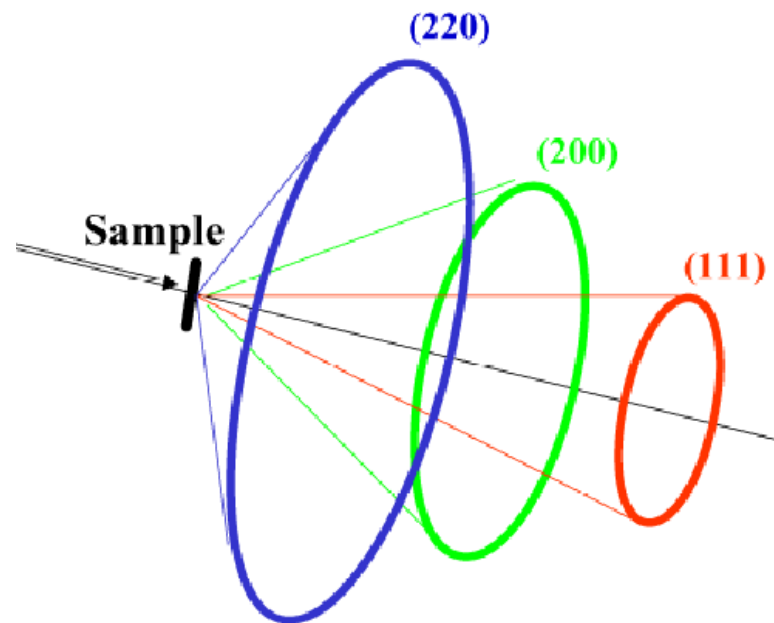
Diffraction from Polycrystals

Debye-Scherrer Cones

- ◆ Crystallites in powder that are in position of reflect diffract into cones of semi-angle $2\theta_{hkl}$ according to Bragg's Law
- ◆ Diffraction occurs only at specific angle represented by the surface of cones (Debye-Scherrer cone)
- ◆ Ewald Construction (?)

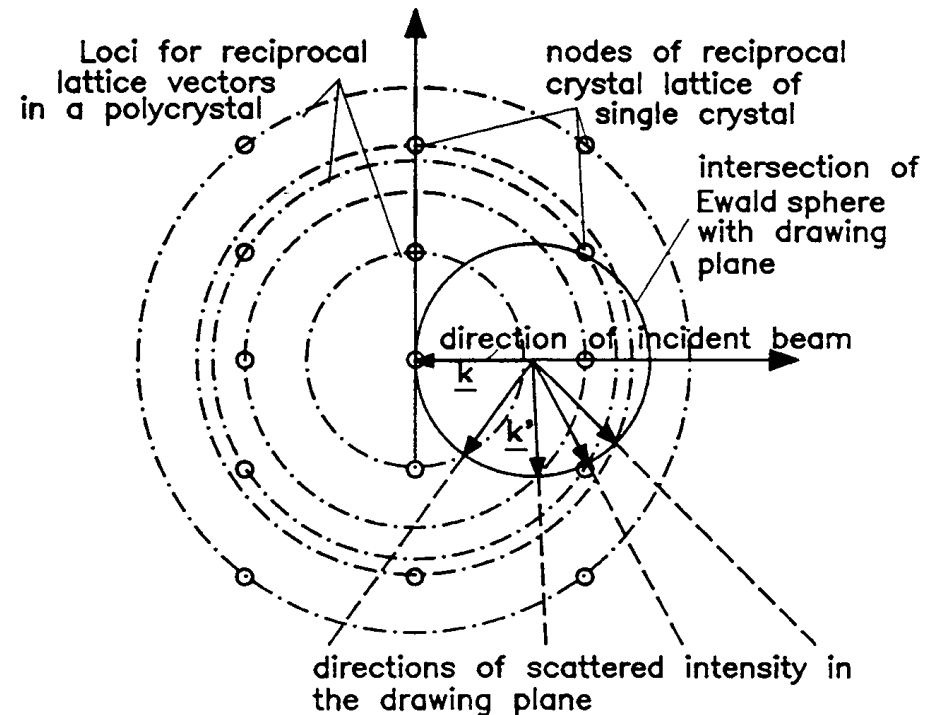


Multiple Crystallites



Diffraction from Polycrystals

- ◆ Polycrystal -- equivalent to spinning reciprocal space
- ◆ Previous discrete allowed directions of \mathbf{K} become circles (Note: $|\mathbf{k}| = |\mathbf{k}'|$)
- ◆ Single crystal must be reoriented to bring various planes (\mathbf{K}) into reflection -- polycrystal remains fixed
- ◆ Varying 2θ brings in reflections
 - Or varying λ at pulse source (varies radius of Ewald sphere)



How are neutrons scattered by atoms (nuclei)?

- ◆ Short-range scattering potential:

$$V(r) = \frac{2\pi\hbar^2}{m} b\delta(r)$$



- ◆ The quantity “b” (or f) is the strength of the potential and is called the scattering length – depends on *isotopic* composition
- ◆ Thus “b” varies over N nuclei – can find average \bar{b}
defines coherent scattering amplitude $b_{coh} = \bar{b}$ leads to diffraction – turns on only at Bragg peaks
- ◆ But what about deviations from average? This defines the incoherent scattering

$$b_{inc} = (\bar{b}^2 - \overline{b^2})^{1/2}$$

- ◆ Incoherent scattering doesn't depend on Bragg diffrac. condition, thus has no angular dependence – leads to background (e.g., H)



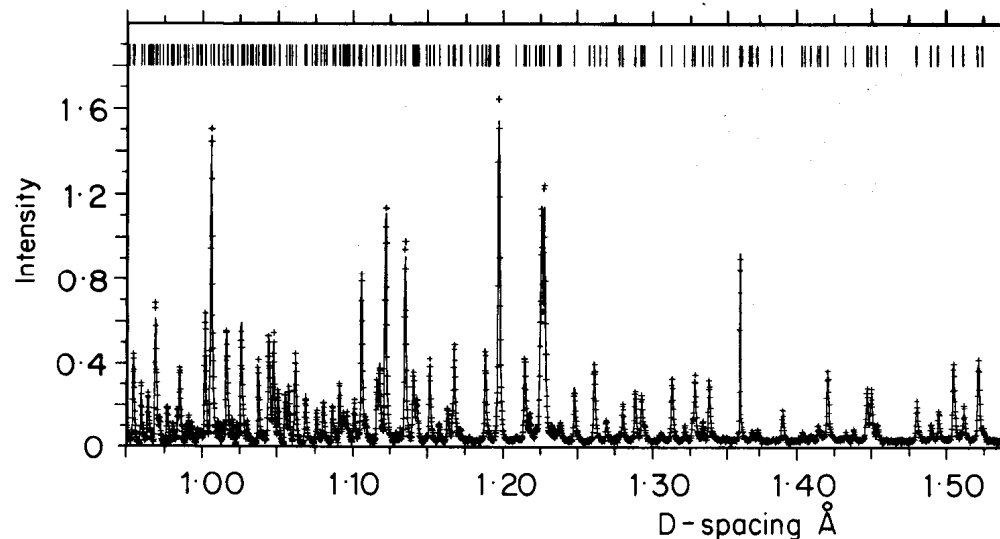
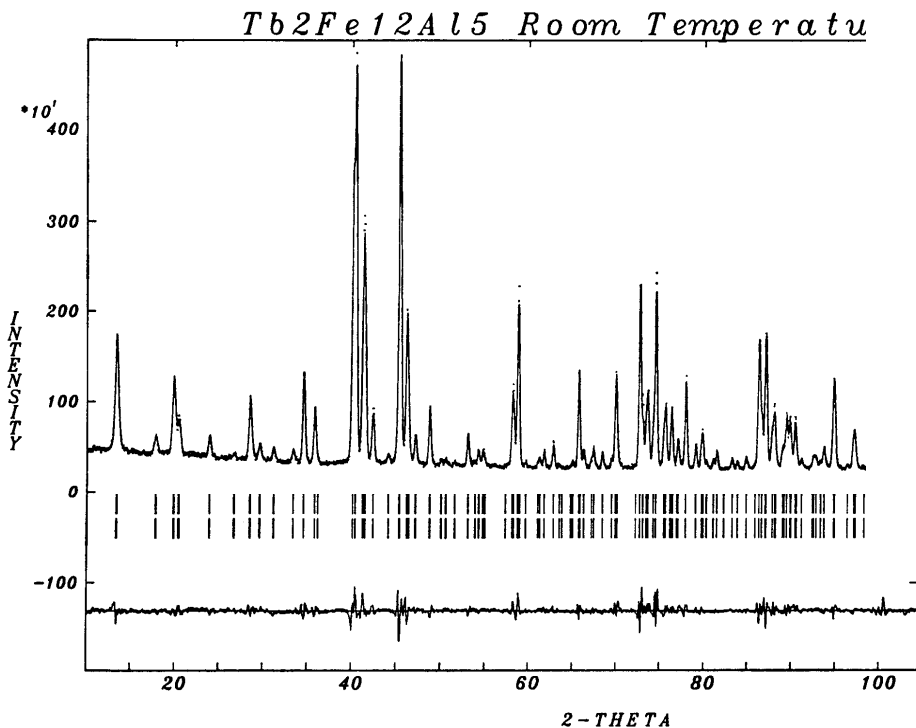
Scattering of neutrons by nuclei

- ◆ A single isolated nucleus will scatter neutrons with an intensity (isotropic)
 - $I = I_0 [4\pi b^2]$
where I_0 = incident neutron intensity, b = scattering amplitude for nucleus
- ◆ What happens when we put nucleus (atom) in lattice?
 - Scattering from N nuclei can add up because they are on a lattice
 - Adding is controlled by phase relationship between waves scattered from different lattice planes
 - Intensity is no longer isotropic – Bragg law gives directional dependence
 - Intensity $I(Q, \text{ or } \theta)$ is given by a scattering cross-section or scattering function

Observed coherent scattering in lattice

- ◆ Intensity of diffracted x-ray or neutron beam produces series of peaks at discrete values of 2θ [or d or K (also Q)]

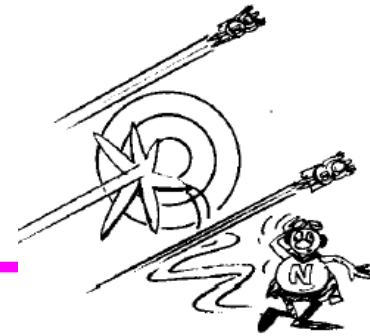
Note: $d = \lambda / (2 \sin\theta)$ or $K = 4\pi \sin\theta / \lambda = 2\pi / d$ are more fundamental since values are independent of λ and thus characteristic only of material.



Benzene Pattern (partial)

Note: Inversion of scales - $2\theta \propto f(1/d)$

Scattering Cross-section



- ◆ The measured scattered intensity in a diffraction experiment is proportional to a scattering function $S(Q)$, which is proportional to a scattering cross-section

$$I(2\theta, d, \text{or } Q) \propto S(Q) \propto \frac{d\sigma}{d\Omega} \quad \Omega = \text{solid angle}$$

- ◆ In turn the cross-section $\propto |A(Q) \cdot A^*(Q)|$

A = scattering amplitude

- ◆ In second Born approximation (kinematic limit) $A \propto$ Fourier transform of scattering length density $\rho(r) = \sum_j \rho_{aj}(\vec{r} - \vec{R}_j)$ (α atom) with the sum over j atoms at position R_j

- ◆ then
$$A(Q) = \sum_j \int \rho_{aj}(r - R_j) e^{2\pi i Q \cdot r} d^3 r = \sum_j f_j(Q) e^{2\pi i Q \cdot R_j}$$

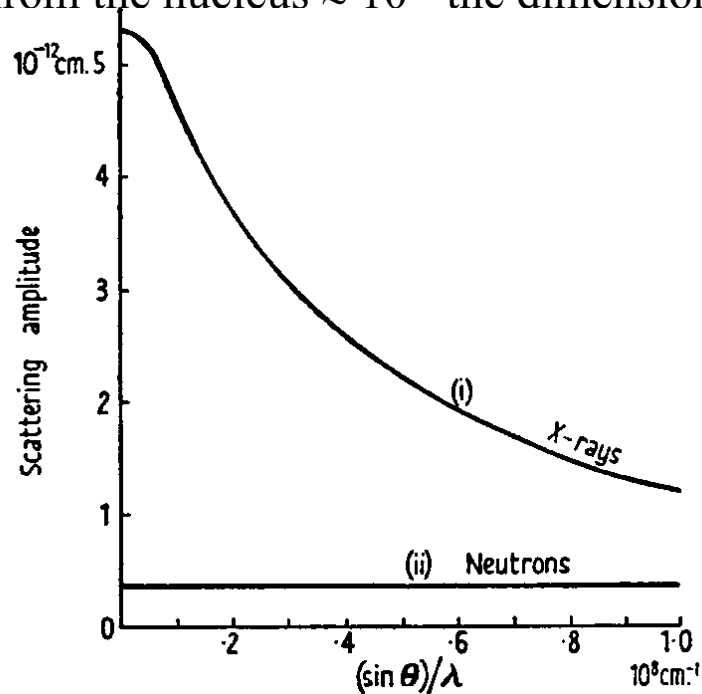
$$\text{where the scattering factor } f_j(Q) = \int \rho_{aj}(r') e^{2\pi i Q \cdot r'} d^3 r'$$

The scattering factor $f(Q)$ is the fundamental quantity describing the scattering of radiation from the material

- f takes different forms depending on the type of radiation
- f varies in magnitude depending on the scattering atom or magnetic spin

Scattering Factors f

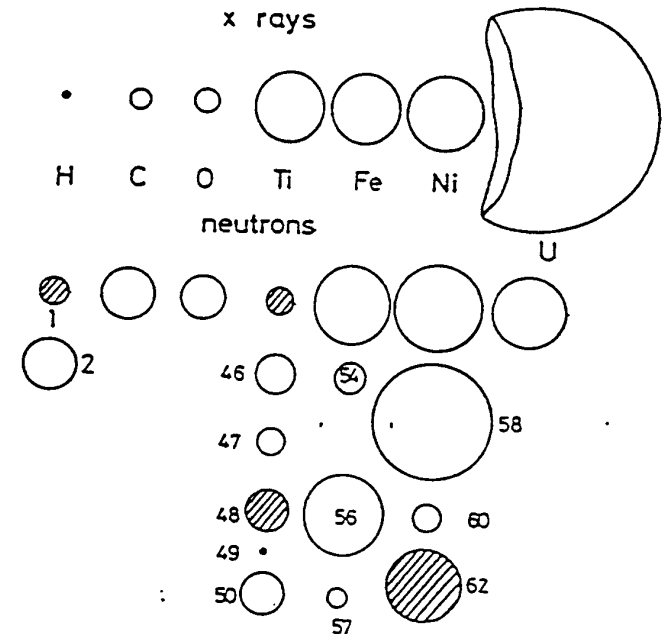
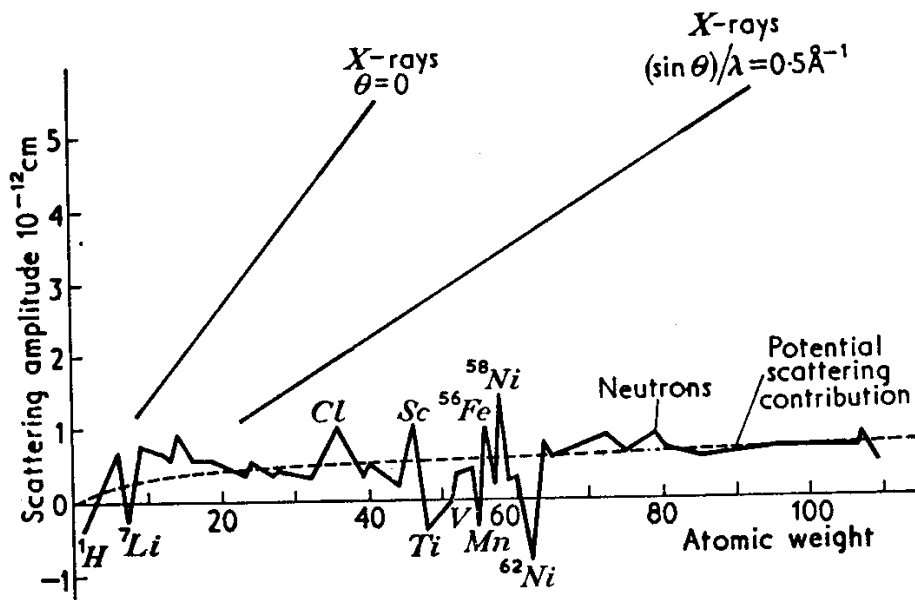
- ◆ The scattering factor $f(Q) = \int \rho_{aj}(r') e^{2\pi i Q \cdot r'} d^3 r'$
- ◆ The Fourier transform character of the scattering factor f means that the radial extent of the scattering center density $\rho_{aj}(r)$ will dictate its Q dependence.
 - x-rays scatter from the electron cloud of dimensions comparable to λ or d ($\propto 1/Q$)
 - Neutrons scatter from the nucleus $\approx 10^{-5}$ the dimension of λ or d



Scattering Factors f , cont'd

- ◆ For x-rays the magnitude of f is proportional to Z
- ◆ For neutrons nuclear factors determine f , thus no regular with Z (different isotopes can have different f s)

RELATIVE SCATTERING FACTORS

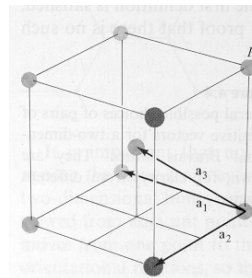
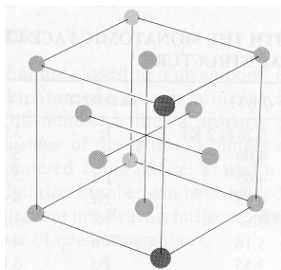


For neutrons conventionally $f = b$
 (Scattering length - constant for an element)

Shaded (negative) $\rightarrow \pi$ phase change

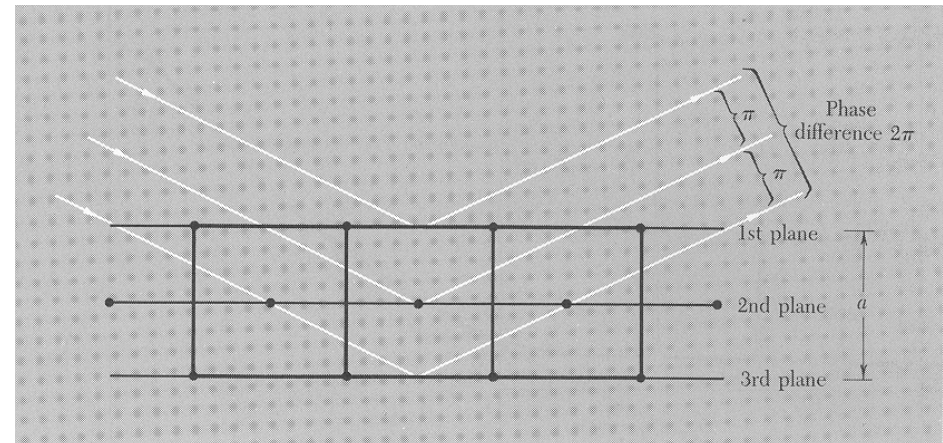
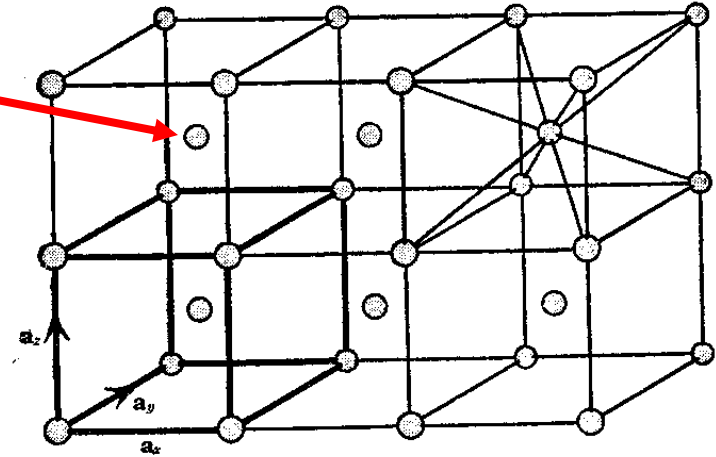
What Controls the Scattering Amplitude?

- ◆ $I(Q) \propto S(Q) \propto |A(Q) \cdot A^*(Q)|$ [Measured scattered intensity, $S = \text{scat.func.}$]
- ◆ $A(Q) = \sum_j f_{aj}(Q) e^{2\pi i Q \cdot R}$ where f_{aj} = atomic scattering factor [cm^{-1}]
- ◆ Magnitude of $A(Q)$ is controlled by $|A(Q) \cdot A^*(Q)|$ called Structure Factor
 - f values for various atoms in lattice
 - destructive interference of waves scattering from atoms at various lattice sites (calculation of above sum over atoms in lattice reveals this)
- ◆ fcc lattice $(000, 0\frac{1}{2}\frac{1}{2}, \frac{1}{2}0\frac{1}{2}, \frac{1}{2}\frac{1}{2}0)$
 - $A(Q) = 4 f_a$ for hkl all odd or hkl all even
 - $A(Q) = 0$ otherwise
- ◆ bcc lattice $(000, \frac{1}{2}\frac{1}{2}\frac{1}{2})$
 - $A(Q) = 2 f_a$ for $h+k+l$ even
 - $A(Q) = 0$ otherwise



Why don't $(h+k+l)$ odd integer index reflections appear for bcc crystals?

- ◆ A bcc cell has an extra plane stuck in between lattice planes separated by a (lattice parameter)
- ◆ Phase difference (path difference) between nearest neighbor planes is π ($\lambda/2$) – destructive interference



And atoms wiggle!

- ◆ Thermal vibration of atoms from their equilibrium position (normal phonon modes) affects the scattering intensity
- ◆ This is represented by the Debye-Waller factor e^{-2W} modifying the scattered intensity, where for a cubic monatomic Bravais lattice

$$2W = \langle (\vec{q} \cdot \vec{u})^2 \rangle = q^2 \langle u_q^2 \rangle \quad u_q^2 = \text{comp. of velocity along } \mathbf{q}.$$

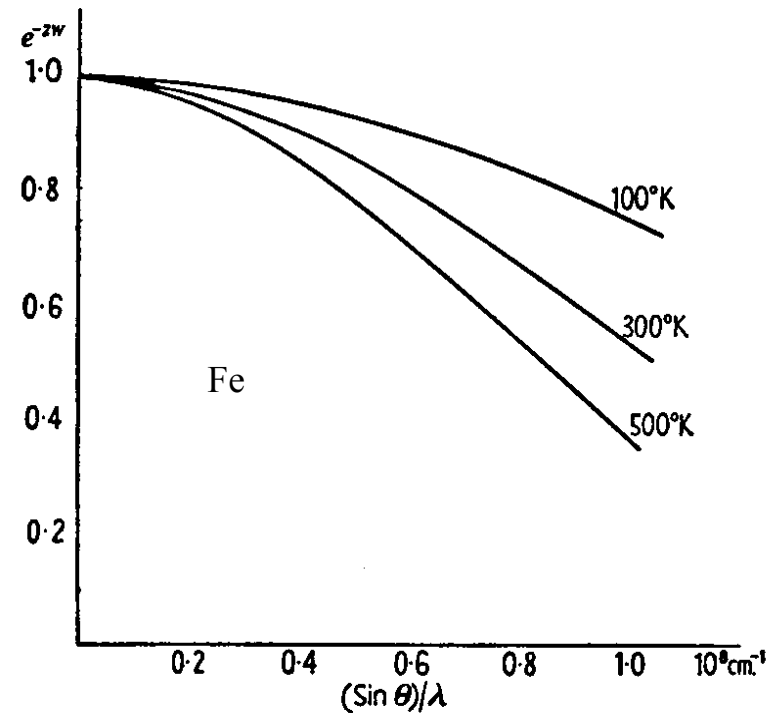
- ◆ In a multi-site lattice each atom may have a unique D-W factor.
- ◆ If the lattice is non-cubic, the velocity components are unequal, and up to 6 components may be required to determine the D-W correction.

Debye-Waller factor temperature and q-dependence

- ◆ Because the D-W factor originates from phonon normal modes, the average velocity is both T- and q-dependent

$$e^{-2W} = e^{-\frac{C}{\theta_D} f\left(\frac{\theta_D}{T}\right) \left(\frac{\sin \theta}{\lambda}\right)^2}$$

Where Θ_D is the Debye temperature from specific heat



Other Factors Affecting Scattering Intensity from Powder

- ◆ $I \propto S(Q) = \lambda^3 [I_o][SF][G][M][TF][LF][AF][PO][EE]|AA^*|$
- I_o = Incident intensity
 - [SF] = Overall scale factor (det. efficiency, everything else you forgot)
 - [G] = Geometrical factors of instrument and sample (e.g., density)
 - [M] = Multiplicity of reflection [# cooperating planes, e.g. 8 (111)]
 - [TF] = Debye Thermal Vibration Factor = e^{-2W}
 - [LF] = Lorenz geometrical factor $LF = 1/(2\sin^2\theta\cos\theta)$ [λ fixed]
 $LF = d^4 \sin\theta$ [TOF]; $LF = 1/\sin^2 2\theta$ [plate geom., λ fixed]
 - [AF] = Absorption factor $AF = e^{-A\lambda}$ [varies as $1/v$] [AF very large for x-rays, small for neutrons except Gd, B, Li, Cd, ...]
 - [PO] = Preferred Orientation factor (compensates for non-random crystallite orientation in sample)
 - [EE] = Primary extinction correction [non-uniform illumination of all reflecting planes]