Neutron and X-ray Scattering Studies of Glass-The basics

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Outline

- Principles of Diffraction
- Diffraction in Crystals: Bragg Peaks
- What Controls the Intensity
- What Happens When There are no Planes
- X-rays and Neutrons
- Elastic vs Total Scattering

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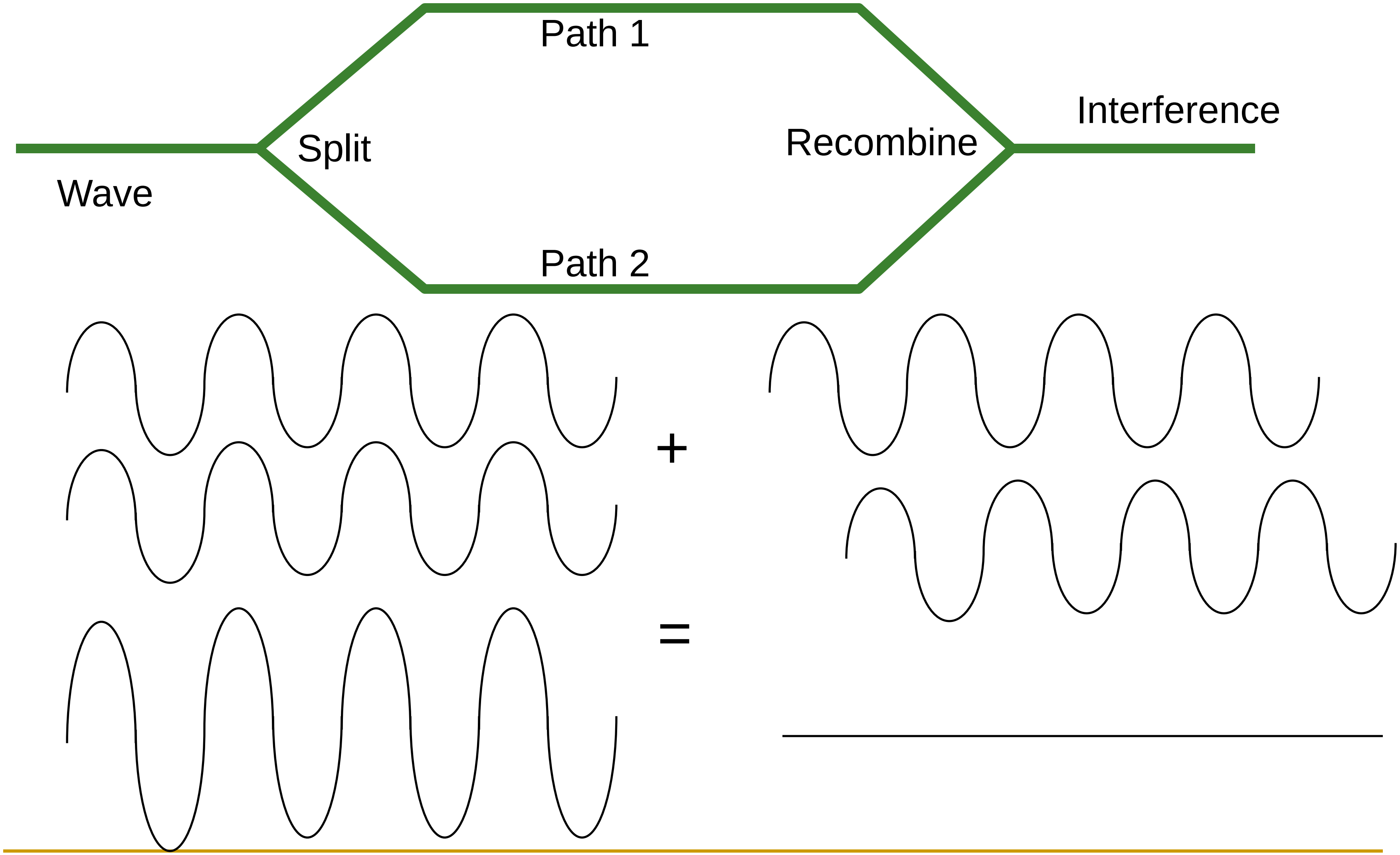
Principle of Diffraction



Path 1

Interference

Split

Recombine

Wave

Path 2

+

=

Resolution

- To use a wave to resolve two features the features must be separated by ≥ the wavelength of the wave
- So the wavelength to resolve features of the order of Å must be of the order of Å (NSOM excepted)
- In E-M radiation that would be X-rays

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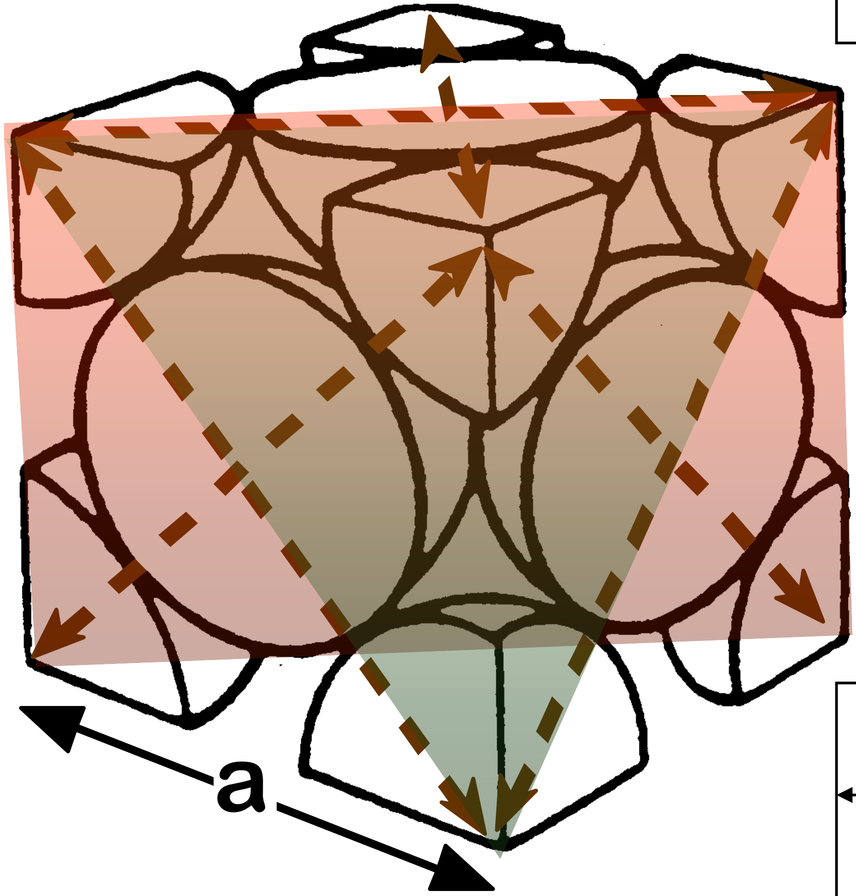
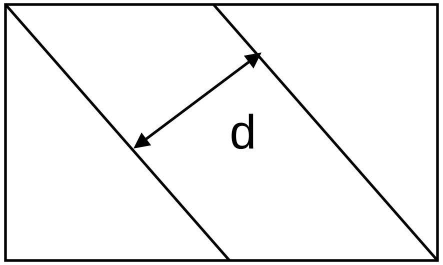
Planes in crystals

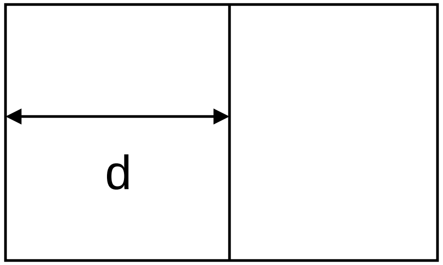


Adapted from Fig. 3.1(a), ***Callister 6e.***

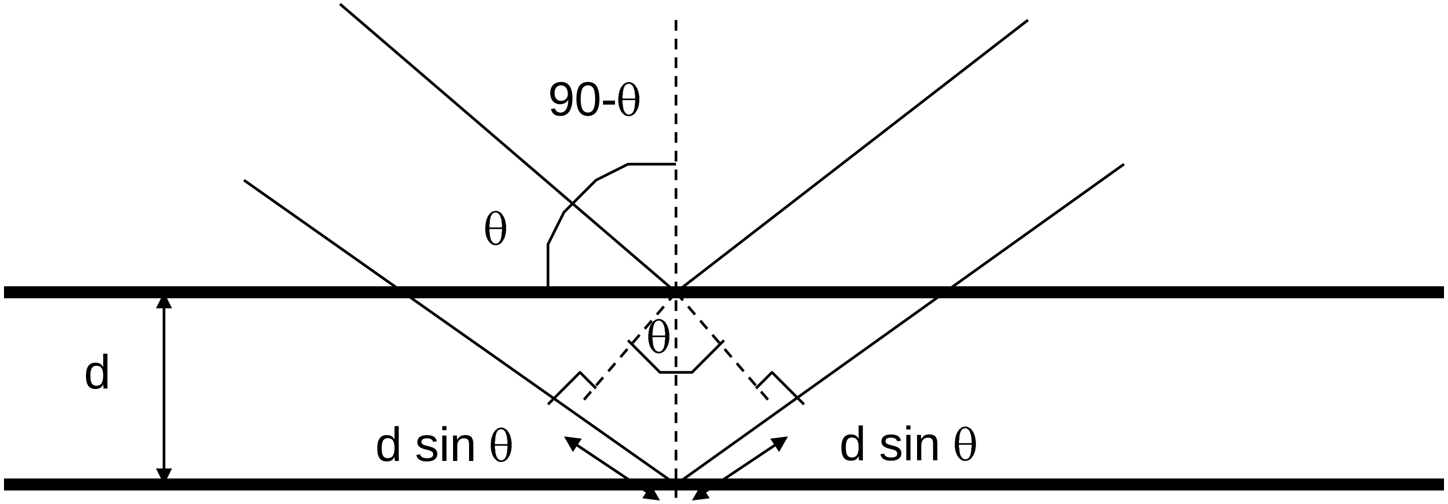


(111) Planes
Projected on
(110) Plane

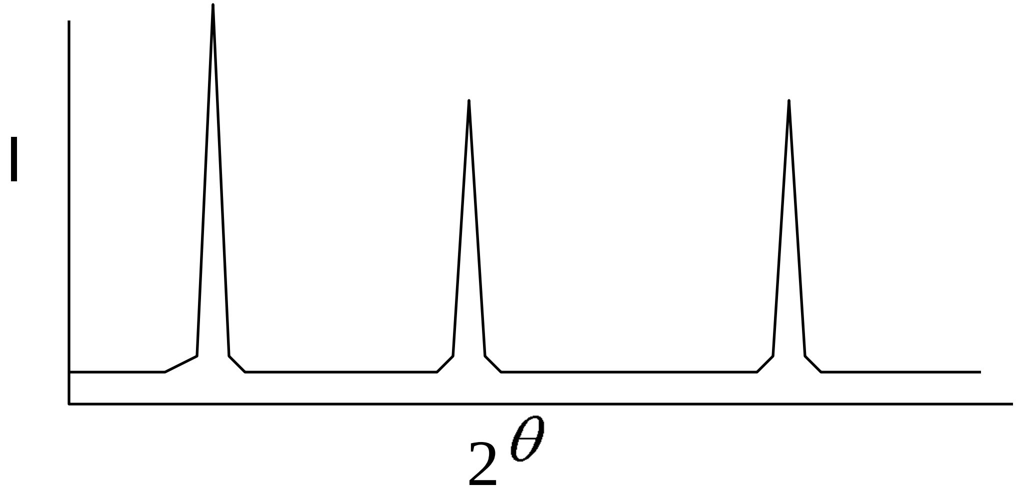
(110) Planes
Projected on
(110) Plane

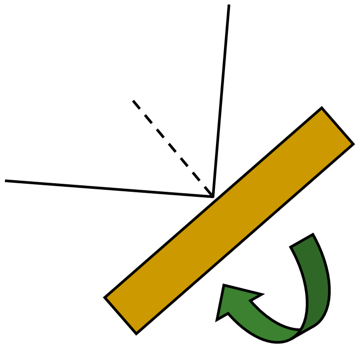


Diffraction from Planes



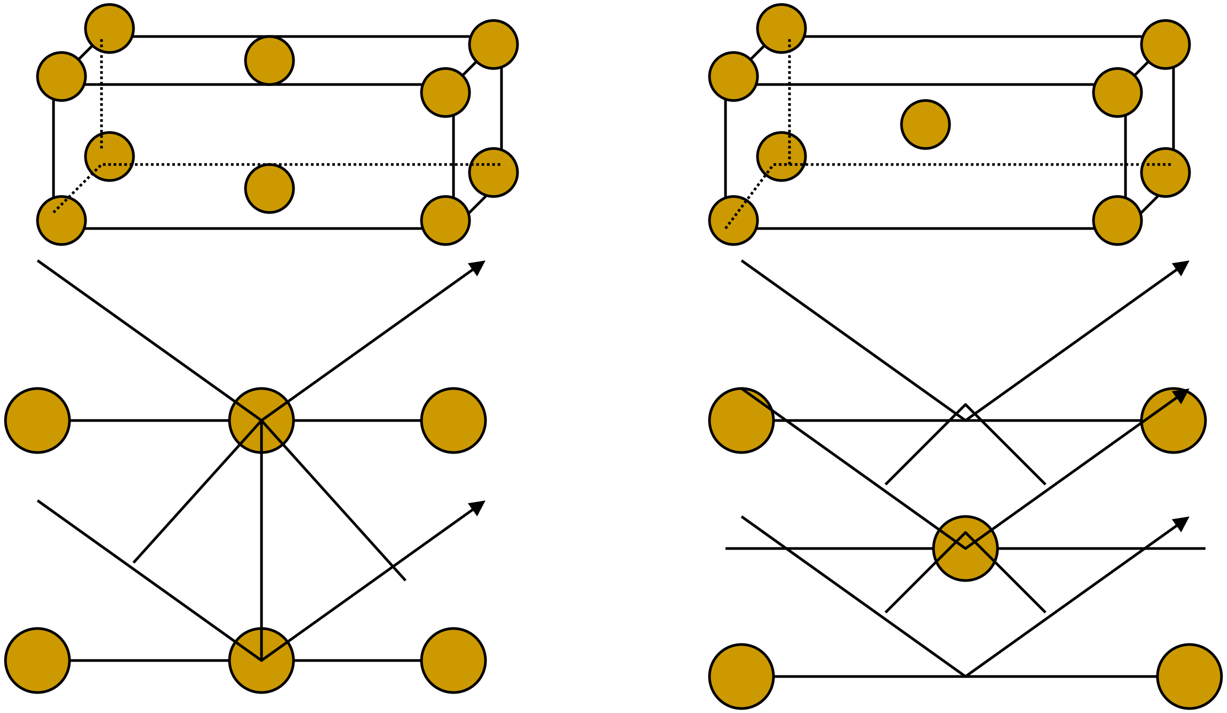
$$2d\sin\theta = n\lambda$$





The d-spacing controls peak position what controls the intensity?

- Atom Position on Planes:



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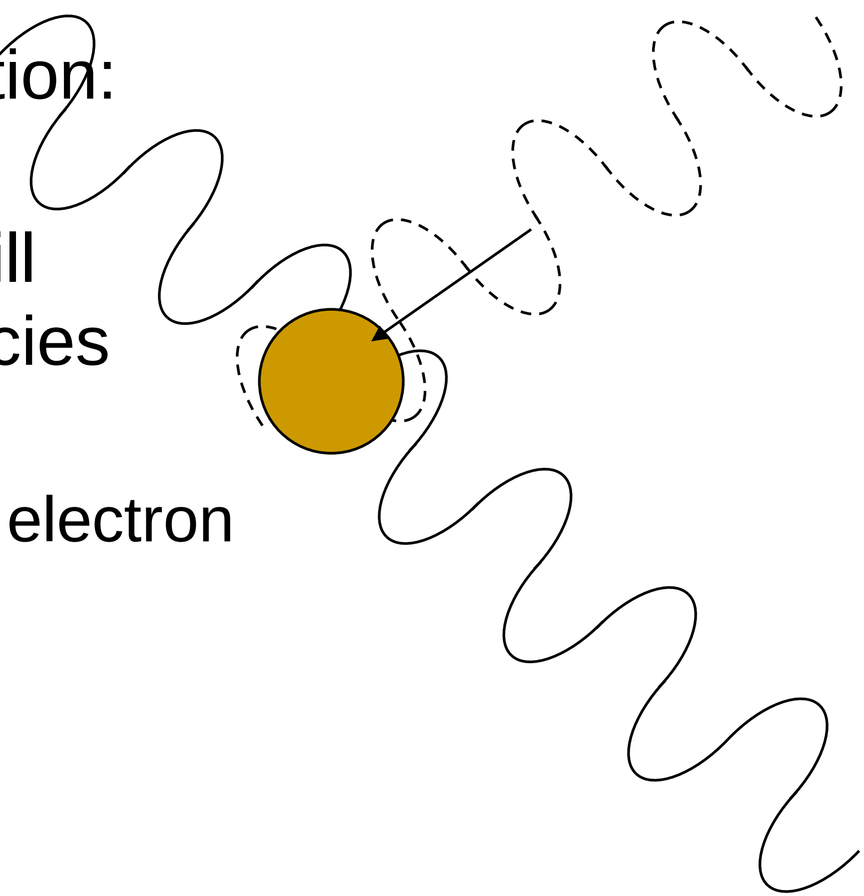
The d-spacing controls peak position what controls the intensity?

- The wave particle interaction: X-rays
- electromagnetic waves will interact with charged species
- Coherent scattering and Compton Scattering (incoherent)
- Phase change of π
- Angular Dependence
- Polarization Dependence

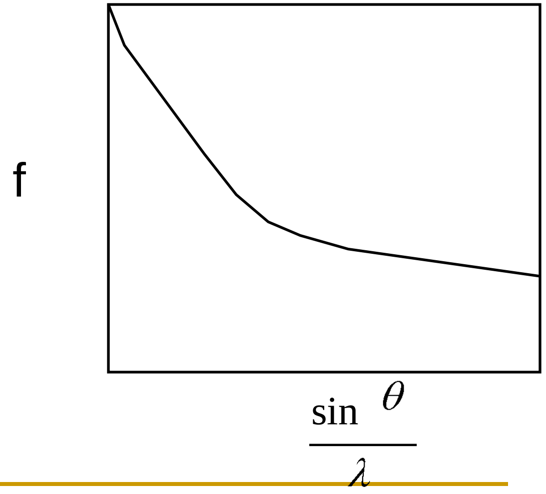


The d-spacing controls peak position what controls the intensity? X-rays

- The wave particle interaction
- Scattering from atom is due to electrons (nucleus too heavy to be oscillated)
- Atomic scattering factor

$$f = \frac{\text{amplitude of wave scattered by an atom}}{\text{amplitude of wave scattered by one electron}}$$

$$f = Z : 2^{\theta} = 0$$



- Form factor depends on distribution of electrons round the nucleus
- Compton increases as Z decreases

The d-spacing controls peak position what controls the intensity? X-rays

- In polycrystalline material the structure factor can be calculated which is a sum of the amplitude and phase of each scattered wave modulated by the form factor for that atom.

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The d-spacing controls peak position what controls the intensity? Neutrons

- The wave-particle interaction is with the NUCLEUS
- Different isotopes have different levels of interaction
- A measure of the level of interaction is called the "cross section" σ and it is measured in "barns" where

$$1 \text{ barn} = 10^{-24} cm^2$$

- It can also be expressed as the scattering length where

$$\sigma = 4 \pi b^2$$

- You can find the neutron cross sections and scattering lengths at

http://www.ncnr.nist.gov/resources/n-lengths/

http://www.ati.ac.at/~neutropt/scattering/table.html

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What does cross section mean?

The d-spacing controls peak position what controls the intensity? Neutrons

Column	Unit	Quantity
1	---	Isotope
2	---	Natural abundance (For radioisotopes the half-life is given instead)
3	fm	bound coherent scattering length
4	fm	bound incoherent scattering length
5	barn	bound coherent scattering cross section
6	barn	bound incoherent scattering cross section
7	barn	total bound scattering cross section
8	barn	absorption cross section for 2200 m/s neutrons

Note: 1fm=1E-15 m, 1barn=1E-24 cm^2, scattering lengths and cross sections in parenthesis are uncertainties.

All of this data was taken from the Special Feature section of neutron scattering lengths and cross sections of the elements and their isotopes in *Neutron News*, Vol. 3, No. 3, 1992, pp. 29-37.

Neutron scattering lengths and cross sections

Isotope	conc	Coh b	Inc b	Coh xs	Inc xs	Scatt xs	Abs xs
Si	---	4.1491	---	2.163	0.004	2.167	0.171
28Si	92.23	4.107	0	2.12	0	2.12	0.177
29Si	4.67	4.70	0.09	2.78	0.001	2.78	0.101
30Si	3.1	4.58	0	2.64	0	2.64	0.107

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The d-spacing controls peak position what controls the intensity? Neutrons

Neutron scattering lengths and cross sections							
Isotope	**conc**	**Coh b**	**Inc b**	**Coh xs**	**Inc xs**	**Scatt xs**	**Abs xs**
Dy	---	16.9-0.276*i*	---	35.9	54.4(1.2)	90.3	994.(13.)
156Dy	0.06	6.1	0	4.7	0	4.7	33.(3.)
158Dy	0.1	6.(4.)	0	5.(6.)	0	5.(6.)	43.(6.)
160Dy	2.34	6.7	0	5.6	0	5.6	56.(5.)
161Dy	19	10.3	(+/-)4.9	13.3	3.(1.)	16.(1.)	600.(25.)
162Dy	25.5	-1.4	0	0.25	0	0.25	194.(10.)
163Dy	24.9	5.0	1.3	3.1	0.21	3.3	124.(7.)
164Dy	28.1	49.4-0.79*i*	0	307.(3.)	0	307.(3.)	2840.(40.)

Note: 1fm=1E-15 m, 1barn=1E-24 cm^2, scattering lengths and cross sections in parenthesis are uncertainties.

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Concept Check

- The position of a “peak” in a diffraction pattern is controlled by the interference between 2 waves scattered from two scattering centers (in the case of a crystalline material this is two crystal planes)
- The intensity of the peak is controlled by
  - The number of scattering centers (in the case of a crystal the number of atoms per unit plane area)
  - The level of interaction between the wave and the scattering center (in the case of a crystal what type of atoms reside on the plane)

Stay Awake Question

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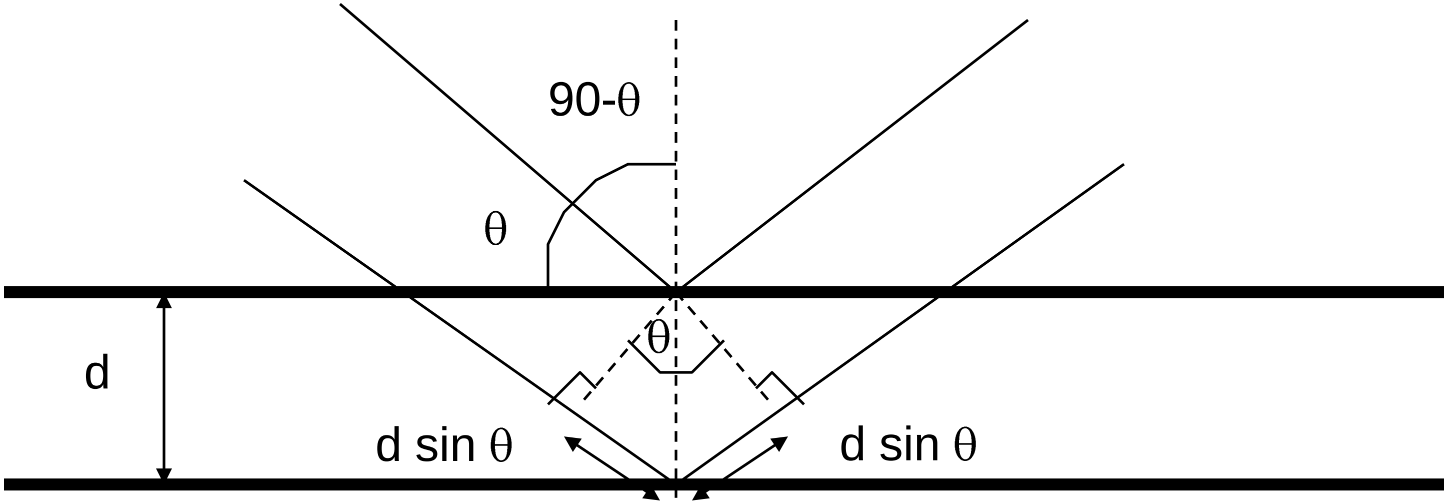
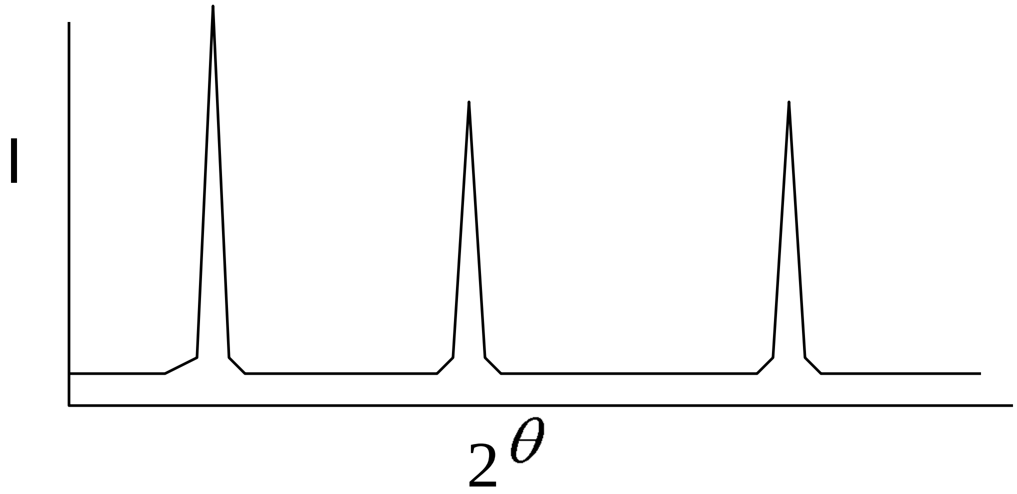
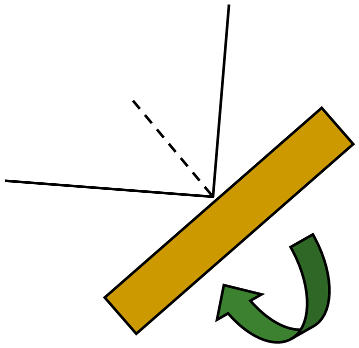
Diffraction from Planes



$$2\left(d\sin\theta\right) = n\lambda$$





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Diffraction by a Polycrystalline Sample

Bragg's law (first order):

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

where λ is the incident wavelength and 2θ is the scattering angle. Rearranging and multiplying through by 2π gives

$$Q \quad = \quad \underbrace{(4\pi/\lambda) \sin\theta}_{\text{Diffraction Variables}} \quad = \quad \underbrace{2\pi/d}_{\text{Sample Parameter}}.$$

To measure the intensity, $I(Q)$, it is possible to:

(i) Vary 2θ at fixed λ.

(ii) Vary λ at fixed 2θ.

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What if there are no planes?

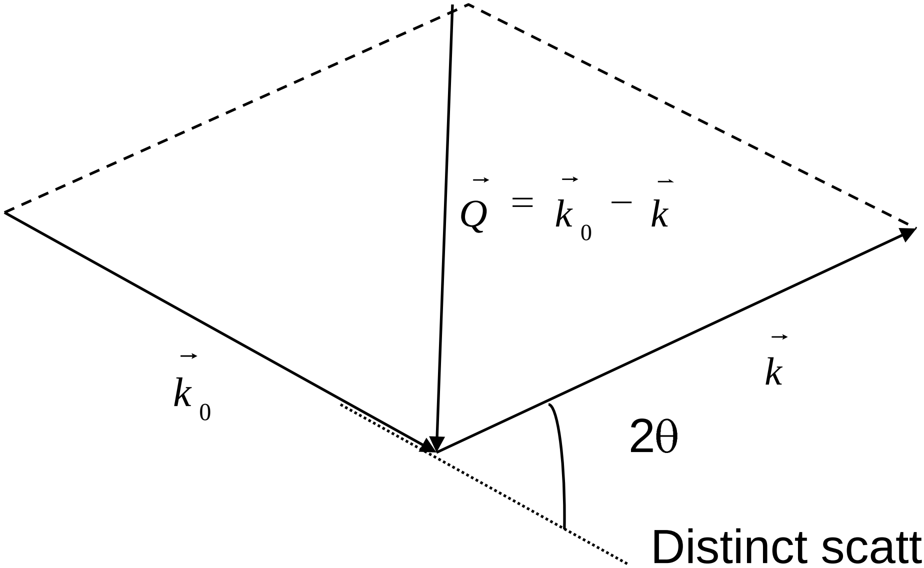
Born Approximation for Scattering Cross Section

A System of Particles :

$$G(\vec{r},t) = G^{S}(\vec{r},t) + G^{D}(\vec{r},t)$$

S = self D = distinct

Self scattering is the correlation between the original scattering center at time=0 and itself at time=t



Distinct scattering is the correlation between the original scattering center at time=0 and a different one at time=t

$$\hbar\omega = E_0 - E \qquad \hbar\vec{Q} = \hbar\vec{k}_0 - \hbar\vec{k}$$

What does that give us?

- Distinct scattering is what we want for structure: it is the spatial distribution of our scattering centers
- Self scattering tells you about dynamics

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Basic Properties of X-rays and Neutrons

Property	X-rays	Neutrons
Wavelength	Ag-Kα to Cr-Kα ,0.56-2.29Å Synchotron tune 0.01Å-123Å	0.8-10Å
Energy at 1Å	≈12.4keV not likely to initiate atomic vibreations	80meV similar to typical phonon energy
Production	X-ray tube, synchotron or X-ray laser	Reactor or pulsed accelerator
Detection	Proportional counters or scintillators	Gas counters or scintillators
Angular dependence	Form factor f(Q)	No Q dependence if non magnetic
Isotopic variation	None	b varies irregularly with Z
Phase change on scattering	180	180 or 0
Magnetic	None	Magnetic form factor

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Where X-rays and Neutrons Differ

- For x-rays the coherent scattering depends on $f(\vec{Q}_0)$ where $\vec{Q}_0$ is the elastic scattering vector, this is roughly proportional to Z. The dimensions of the atomic orbitals are similar to the wavelength of the X-rays. While interaction with phonons are small, interaction with electron momentum (Compton Scattering) is large (this can be used-see later)
- For Neutrons the scattering length of an electron is small so nuclear scattering dominates (unless there is magnetic scattering (see later) The scattering length is not Q dependent (nucleus is too small) it does not vary systematically with atomic number. The inelastic scattering of neutrons can be used to determine phonon distributions (see later)

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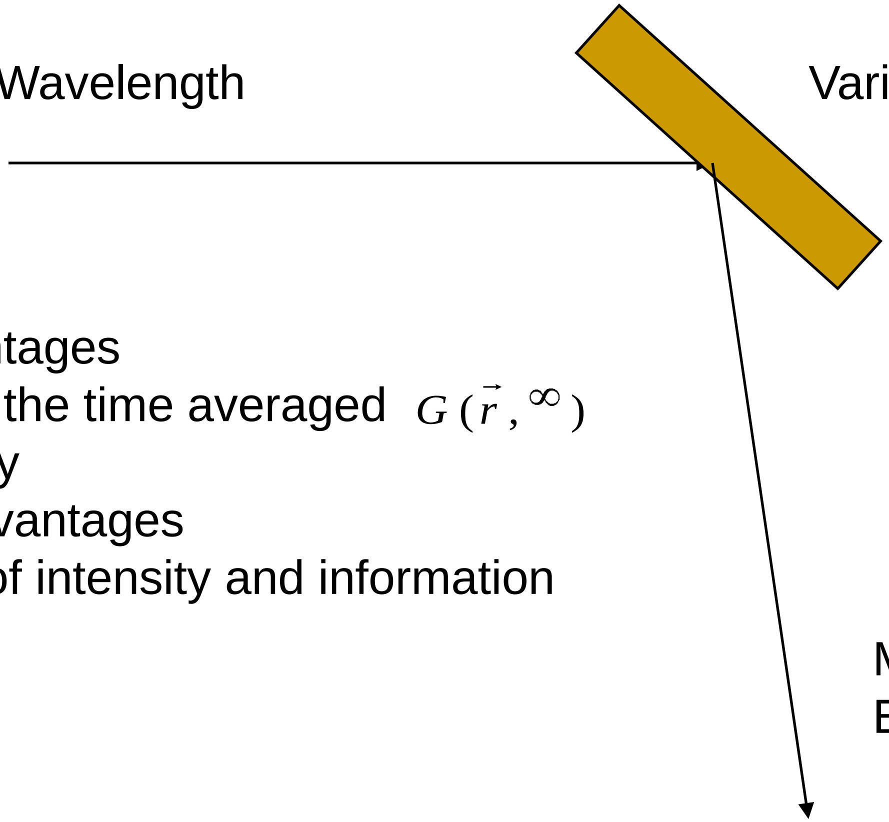
Elastic Scattering



Single Wavelength

Variable angle

Monochromate or
Energy analyze

Advantages

Gives the time averaged $G(\vec{r}, \infty)$ directly

Disadvantages

Loss of intensity and information

Total Scattering for Neutrons

- All neutrons scattered at a given angle are measured

$$\frac{d\sigma}{d\Omega}$$

- Where Ω is the solid angle into which the neutrons are scattered and N_u is the number of composition units

$$\frac{1}{N_u}\frac{d\sigma}{d\Omega} = I_N\left(\vec{Q}_0\right) = I_N^{coh}\left(\vec{Q}_0\right) + I_N^{incoh}\left(\vec{Q}_0\right)$$

$$= \sum_j \bar{b}_j^{\,2} + \sum_j \sum_k \bar{b}_j \bar{b}_k \infty \int_o^\infty 4\pi r^2 \rho_{jk}\left(r\right) \frac{\sin Q_0 r}{Q_0 r}\, dr$$

What is it we want?

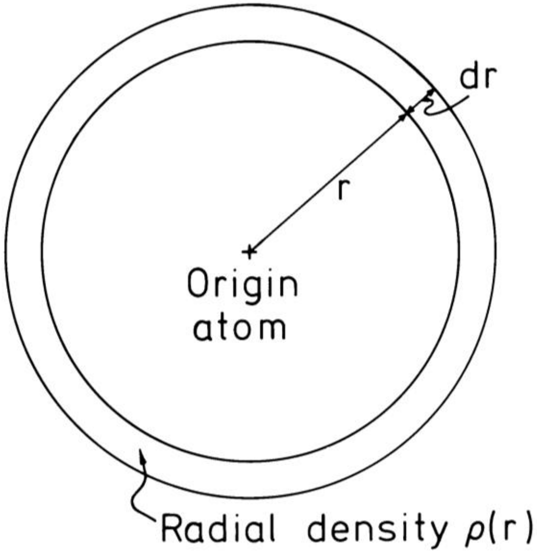
- The best that we can do it to be able to get at the function $\rho(r)$ which we can interpret through the correlation functions :

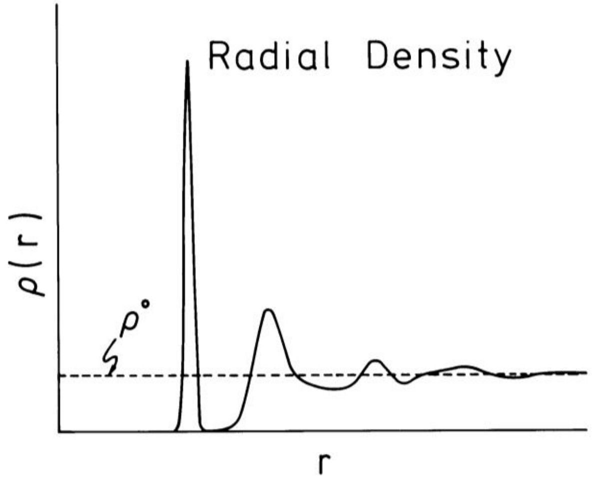
$$g(r) = 4\pi r^2 \rho(r)$$

$$d(r) = 4\pi r\left[\rho(r) - \rho_0\right]$$

$$t(r) = 4\pi r \rho(r)$$

Radial Density Function





$\rho(r)$ is the radial density function and is equal to the average number of atoms per unit volume at a distance r from an arbitrarily chosen origin atom.

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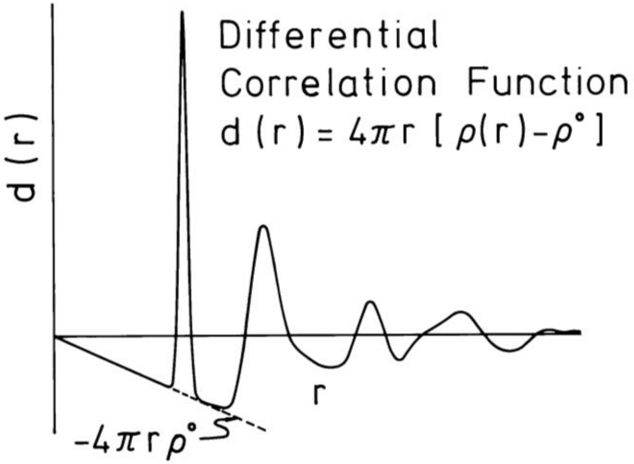
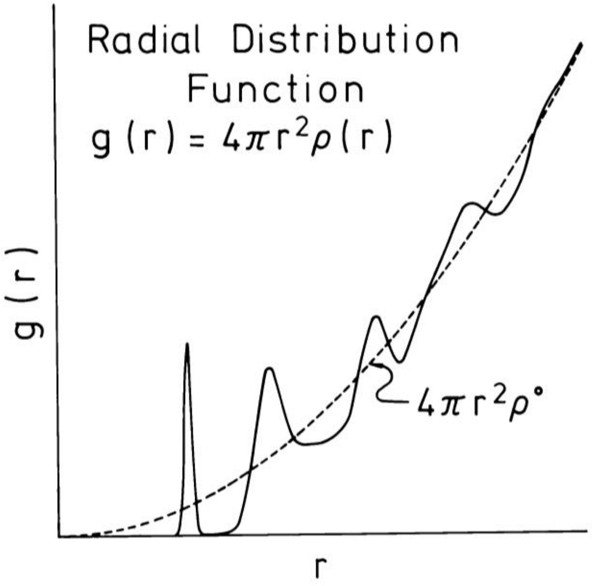
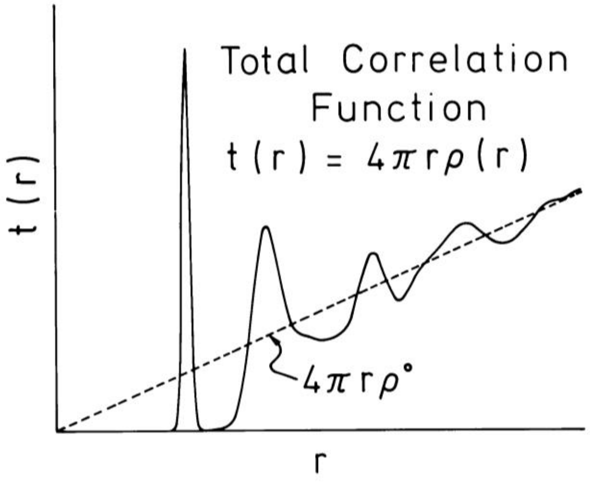
Real Space Correlation Function

Older papers present data as the radial distribution function, whereas modern studies employ the differential correlation function, *d*(*r*), or the total correlation function, *t*(*r*).

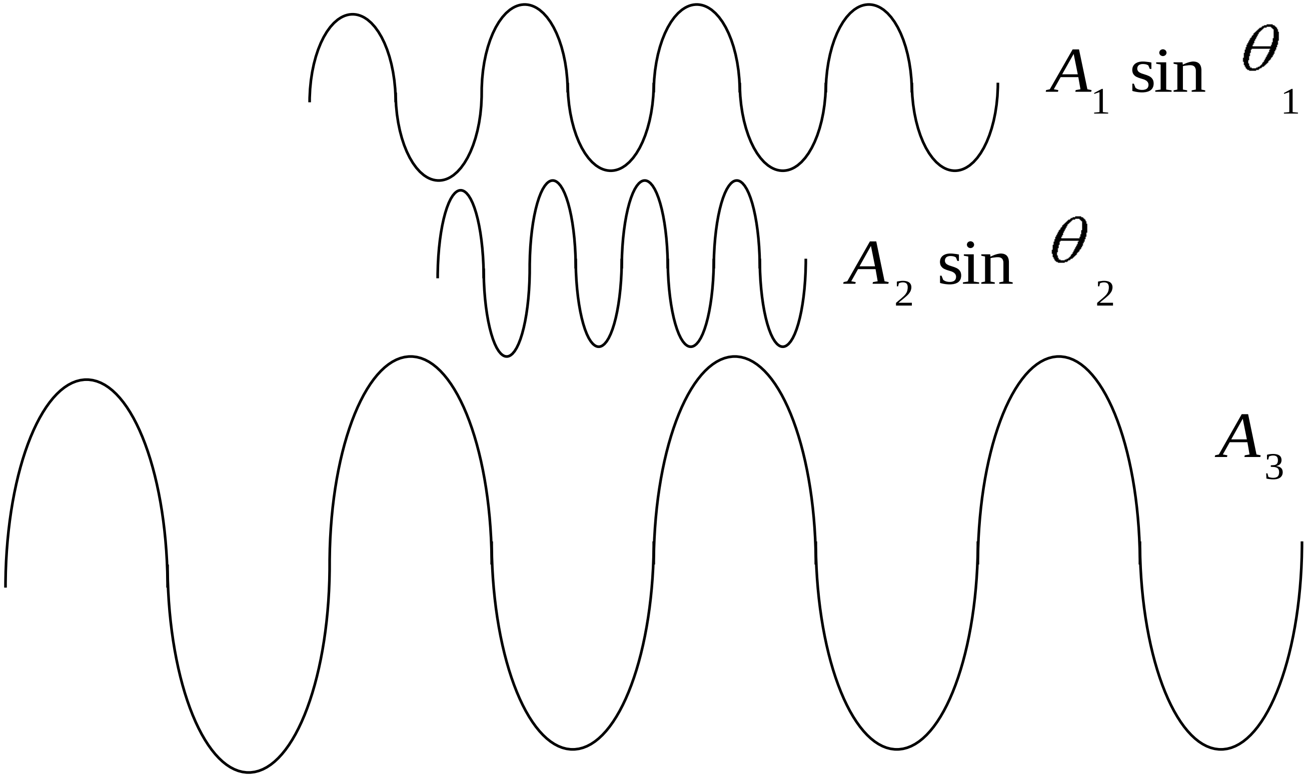






Ya can’t git there from here

- The intensity represents a superposition of sinusoidal waves resulting from pair correlations throughout the structure:



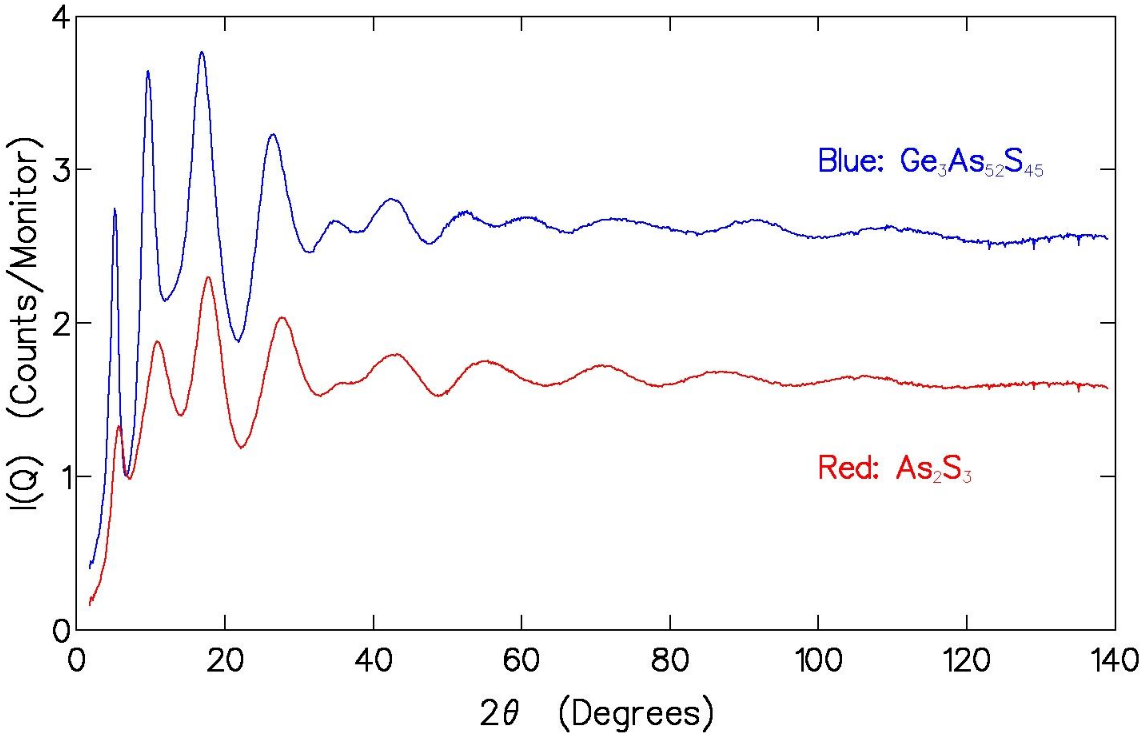
$A_1 \sin \theta_1$

$A_2 \sin \theta_2$

$A_3 \sin \theta_3$

Ya can't git there from here

- So they all add up to some curious looking function

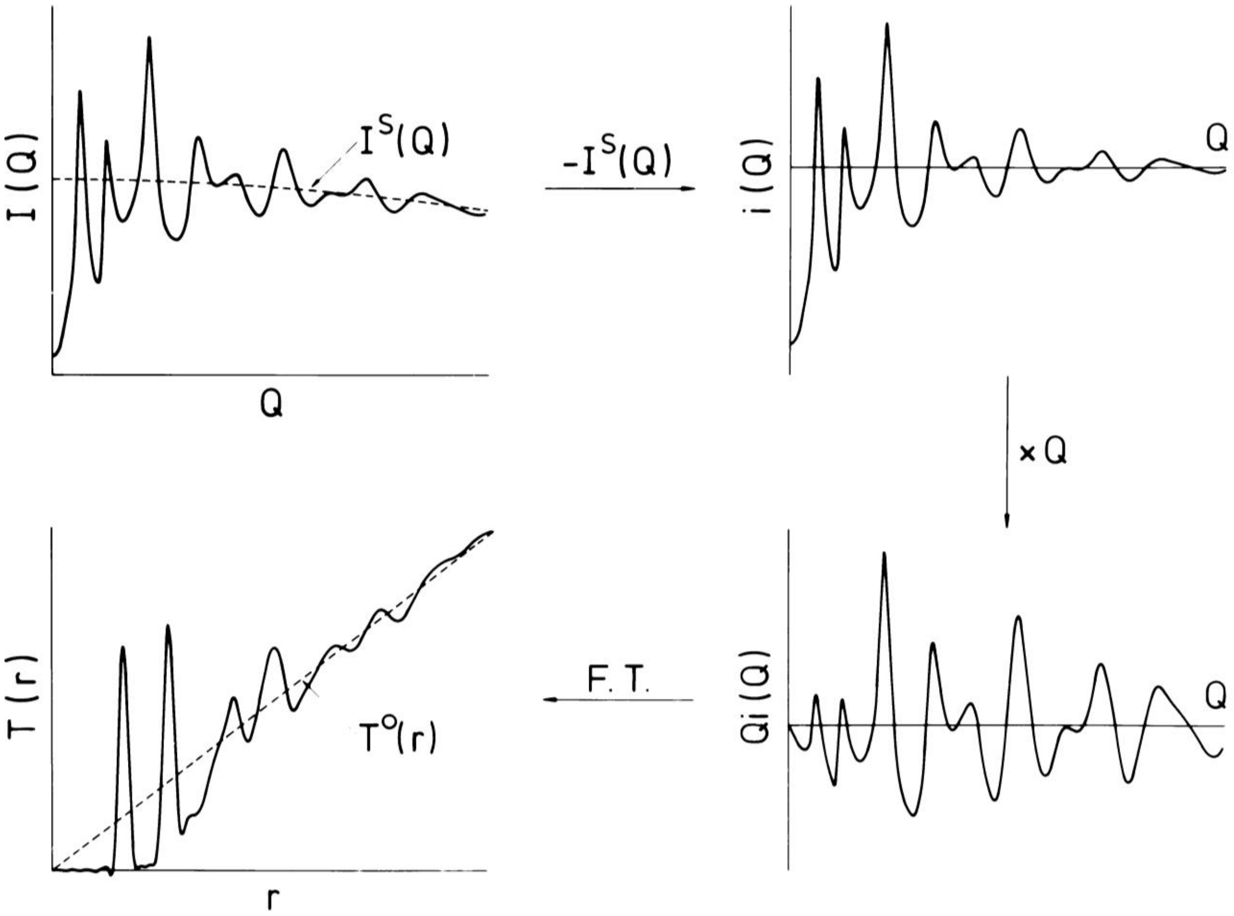


Ya can’t git there from here

- The best way to sort out what frequencies and amplitudes you have in a bunch of sinusoidal waves is to do a Fourier Transform
- A Fourier Transform catalogs the common sin waves in reciprocal space and translates them to a “histogram” in real space

T(*r*) from a Neutron Diffraction Experiment

$$\underset{\text{self}}{I(Q) = I^S(Q)} + \underset{\text{distinct}}{i(Q)}$$



$$T(r) = T^o(r) + \frac{2}{\pi}\int_0^\infty Qi(Q)\,M(Q)\sin rQ\,dQ$$

You can't get to Infinity from Here Either

- Why do we Fourier Transform Qi(Q)?
- Truncation of the Fourier Integral
- How the way you truncate affects your real space correlation function
- How high should you go in Q anyway?

Truncation of the Fourier Integral

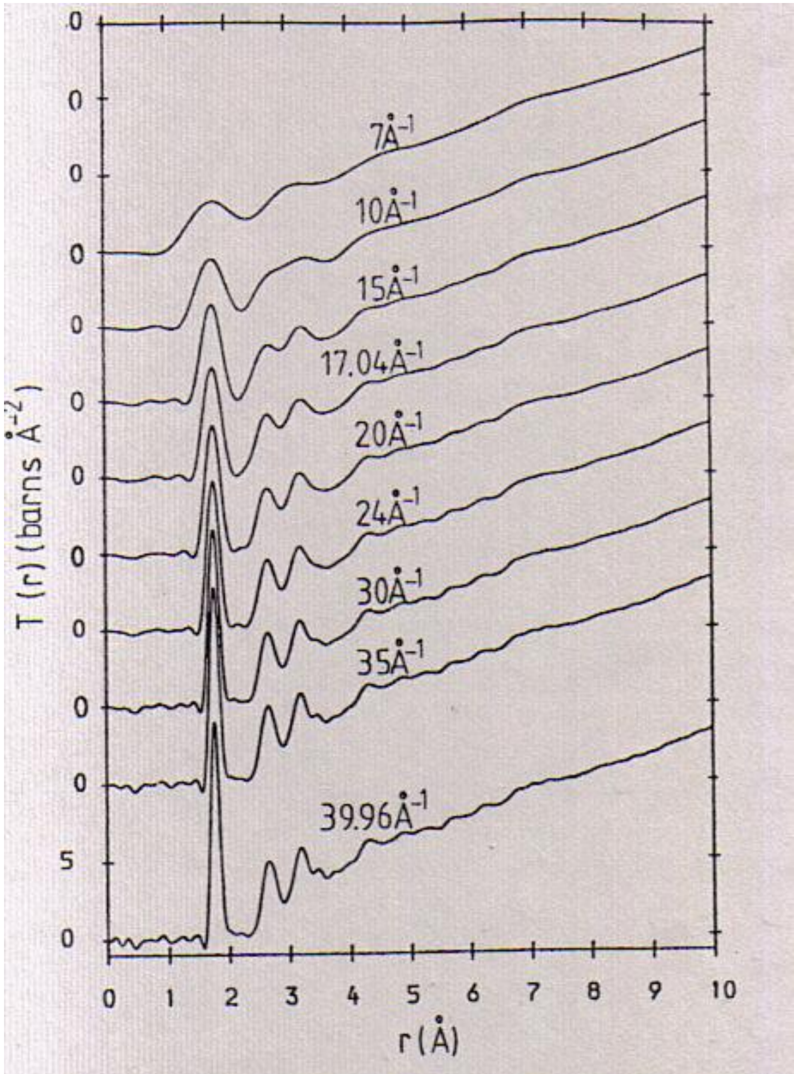


FIGURE 6.7 The Dependence of T(r) Upon Truncation of the Scattering

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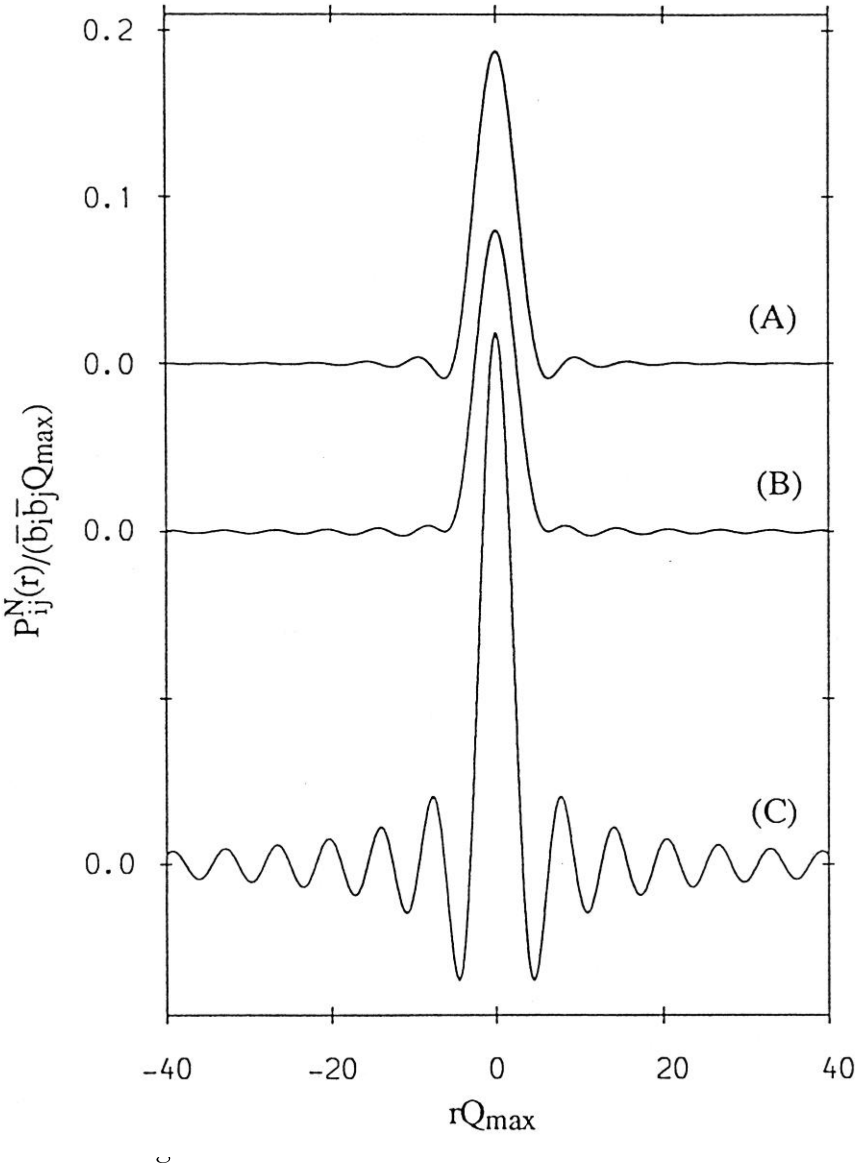
Neutron Peak Function

The termination of the Fourier integral at a finite value of Q, Q_{max}, means that the correlation function is broadened by the real space peak function, $P(r)$. The form of $P(r)$ depends on the modification function, $M(Q)$:

A: Lorch function.

B: Artificial temperature factor.

C: Step function.



Neutron Diffraction Techniques