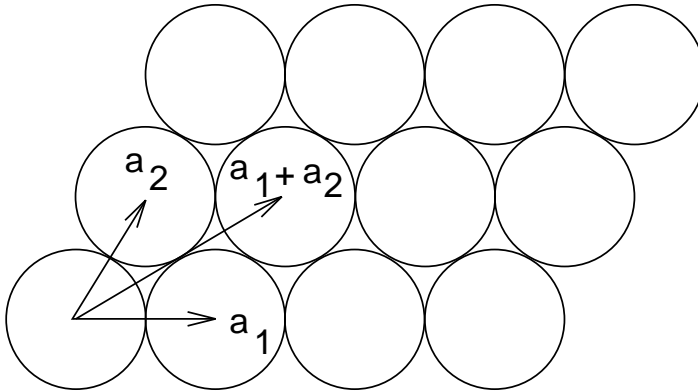


Physics 0551 Lecture #2

Recall from last time the various crystal classes and the different translational and rotational symmetry operations which made this enumeration possible.

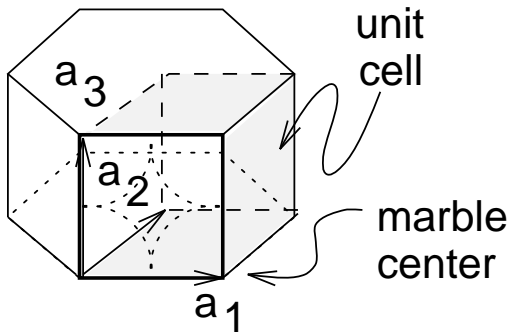
You should also be familiar with the distinction between the CONVENTIONAL and the PRIMITIVE unit cells. (Refer to the 2-D Centered Rectangular Bravais Lattice.)

Example: Consider the 2-D close-packed structure formed by a uniform collection of marbles.



For this system a “hexagonal” lattice (lattice vectors \vec{a}_1 and \vec{a}_2) is formed with a single “marble” per unit cell. Notice that the Wigner-Seitz cells form hexagons.

If identical 2-D planes of marbles are placed directly on top of one another, a simple (primitive) hexagonal 3-D lattice is formed.



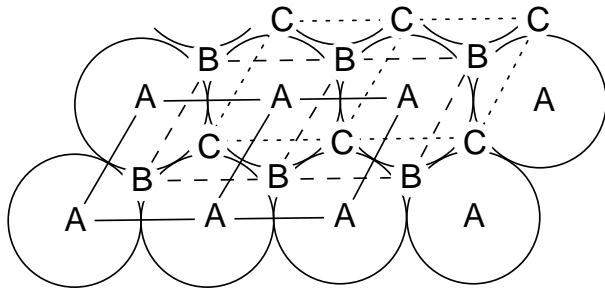
In this case

$$|\vec{a}_1| = |\vec{a}_2| = |\vec{a}_3| \quad \gamma = 60^\circ, \alpha = \beta = 90^\circ$$

Note: this system is no longer close-packed. Let us define this stacking as A/A/A.

Simple Hexagonal (one marble basis)

Looking back at our 2-D hexagonal planes, notice that marbles could be packed more tightly if the marbles are displaced $\frac{1}{3}(\vec{a}_1 + \vec{a}_2)$ (denoted by B's) or $\frac{2}{3}(\vec{a}_1 + \vec{a}_2)$ (denoted by C's) from one layer to the next so that the marble in the next layer reside in the hollows forms by three neighboring marble in the A layer.



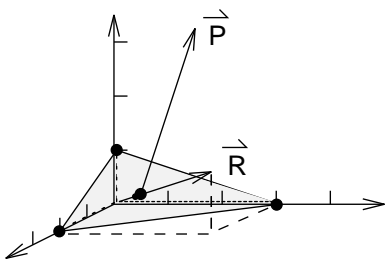
Notice that the B's and C's themselves form a hexagonal 2-D lattice.

Now assume that the first two layers stack A to B. For the third layer, either A or C translations (assume close-packing) are now possible. If the stacking is ABABA....., the *hexagonal close packed* structure (HCP) has been formed. It has a hexagonal 3-D lattice and a two marble basis $|\vec{a}_1| = |\vec{a}_2|$, $|\vec{a}_3| = \sqrt{8/3} |\vec{a}_1|$, $\gamma = 60^\circ$, $\alpha = \beta = 90^\circ$ with marble 1 at $(0,0,0)$ and marble 2 at $(\frac{1}{3}, \frac{1}{3}, \frac{1}{2})$ in terms of $(\vec{a}_1, \vec{a}_2, \vec{a}_3)$. If instead the stacking is ABCABC....., we have a primitive rhombohedral lattice with a single atom basis $|\vec{a}_1| = |\vec{a}_2| = |\vec{a}_3|$ and $\alpha = \beta = \gamma = 60^\circ$. Alternately, we could form a hexagonal unit cell with a 3 marble basis.

In addition, this packing is also the same as the conventional face-centered cubic structure (FCC) which has a cubic unit cell and a **four** atom basis!

Question: How are directions in the “real” space lattice designated?

For this, a common notation of $[u \ v \ w]$ in brackets is used to select a real space vector $\vec{R} = u \vec{a}_1 + v \vec{a}_2 + w \vec{a}_3$.



\vec{P} is perpendicular to the plane formed by the $[3 \ 2 \ 1]$ lattice vector

$$\vec{R} = 3 \vec{a}_1 + 2 \vec{a}_2 + \vec{a}_3$$

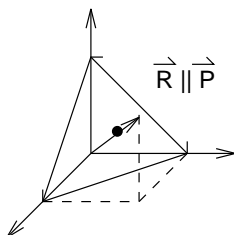
Notice that we form a plane which intercepts the axes at said

points. How do we describe the plane?

$$\left(\frac{1}{u} \ \frac{1}{v} \ \frac{1}{w}\right) \times \text{Lowest Common Denominator}$$

$$\left(\frac{1}{3} \ \frac{1}{2} \ 1\right) \times 6 = (2 \ 3 \ 6)$$

Example: Cubic lattice using $[3 \ 2 \ 1]$



For **cubic** symmetry $[111] \perp (111)$. In general, this is NOT true.

Experimental Methods

Now that we have defined a system of crystals, it is important to develop a series of experimental procedures in order to study “real” crystals.

For this there are a wide variety of techniques to study surfaces and the bulk.

“Real” space images → Transmission electron microscopy (TEM)

Scanning tunneling microscopy (STM)

Diffraction Images → X-ray diffraction, neutron scattering

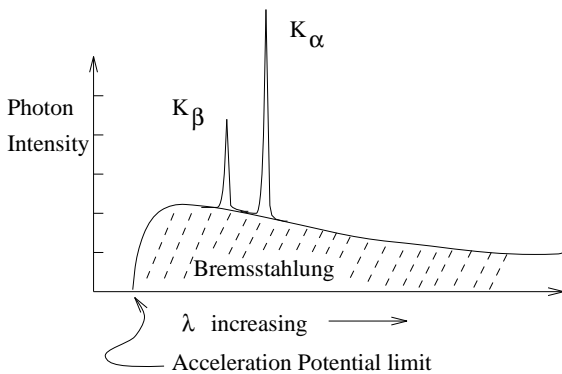
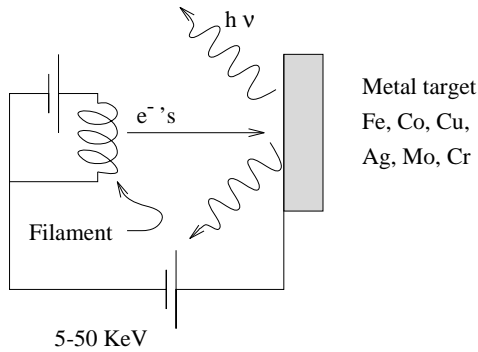
Low energy electron diffraction (LEED)

We will discuss diffraction techniques:

Sources of x-rays - conventional, synchrotron

Sources of neutrons - reactors, spallation

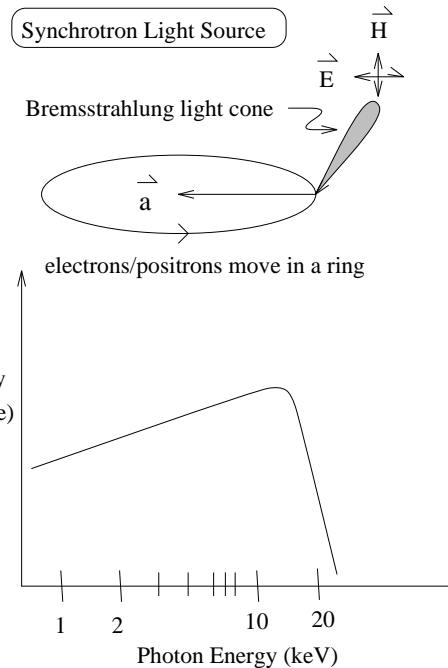
Conventional x-ray source



Two types of radiation:

1. Bremsstrahlung - “de”acceleration of incident e’s
2. Characteristic line spectra - photons from atomic transition $n=2$ to 1 K_{α} $n=3$ to 1 K_{β}
However, the incident e’s must excite $1s$ electrons to the first allowable transition.

Synchrotron Light Source

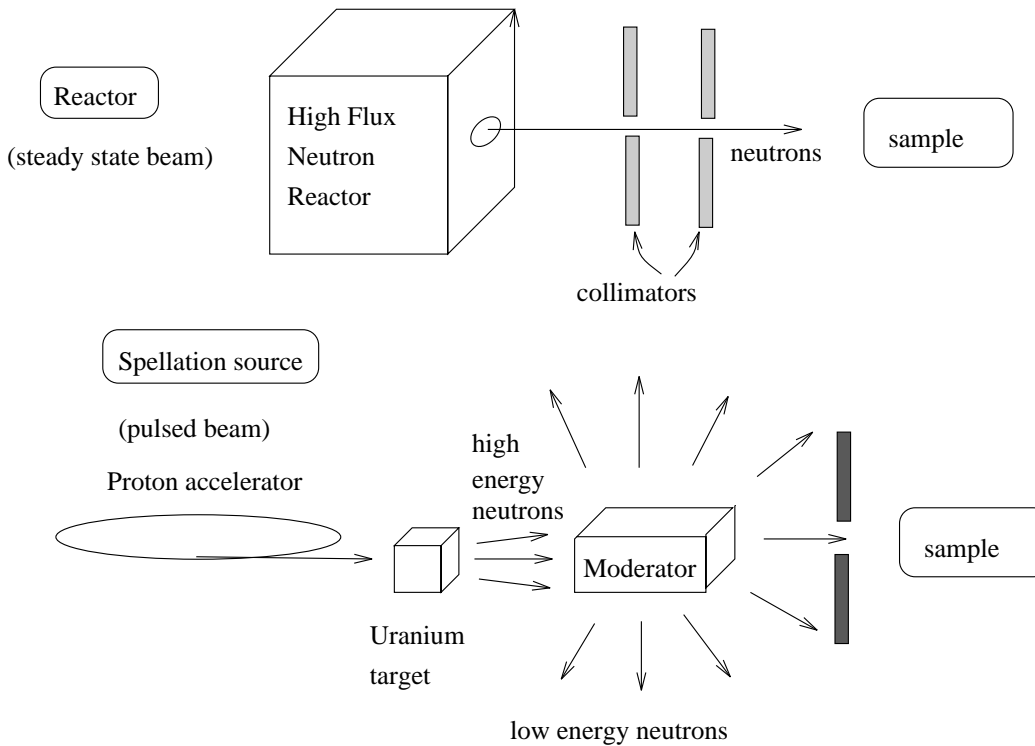


Neutrons:

Reactor - Thermal neutrons from fission events

$$E_{neutron} = 0.025 \text{ eV} = 25 \text{ meV} \quad \lambda \sim 1.5 \text{ \AA}$$

Spallation - High energy protons impinge on a uranium pile.

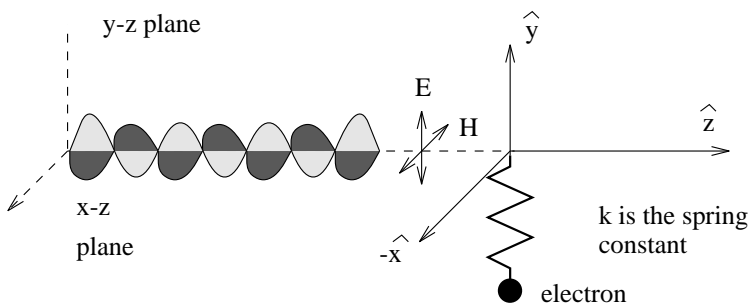


Scattering of x-rays:

This can be solved classically by using Maxwell's equations, or quantum mechanically. In either case the calculation is involved, and will not be reproduced here. (See e.g., X-Ray Diffraction, Azaroff, Kaplow, Kato, Weiss, Wilson, Young.)

The J. J. Thomson model of scattering due to acceleration of the electrons follows.

The incident photon $\vec{E} = \vec{E}_0 \exp\{i(\omega t - kz)\}$, can be described as a travelling wave and the electron is considered to be fixed by an attached spring with spring constant K .



$$\vec{F}_e = e[\vec{E} + \frac{1}{c}(\dot{\vec{x}} \times \vec{H})] - k\vec{x}$$

$$m\ddot{\vec{x}} = e\vec{E} - k\vec{x} \quad \omega_0 = \sqrt{k/m}$$

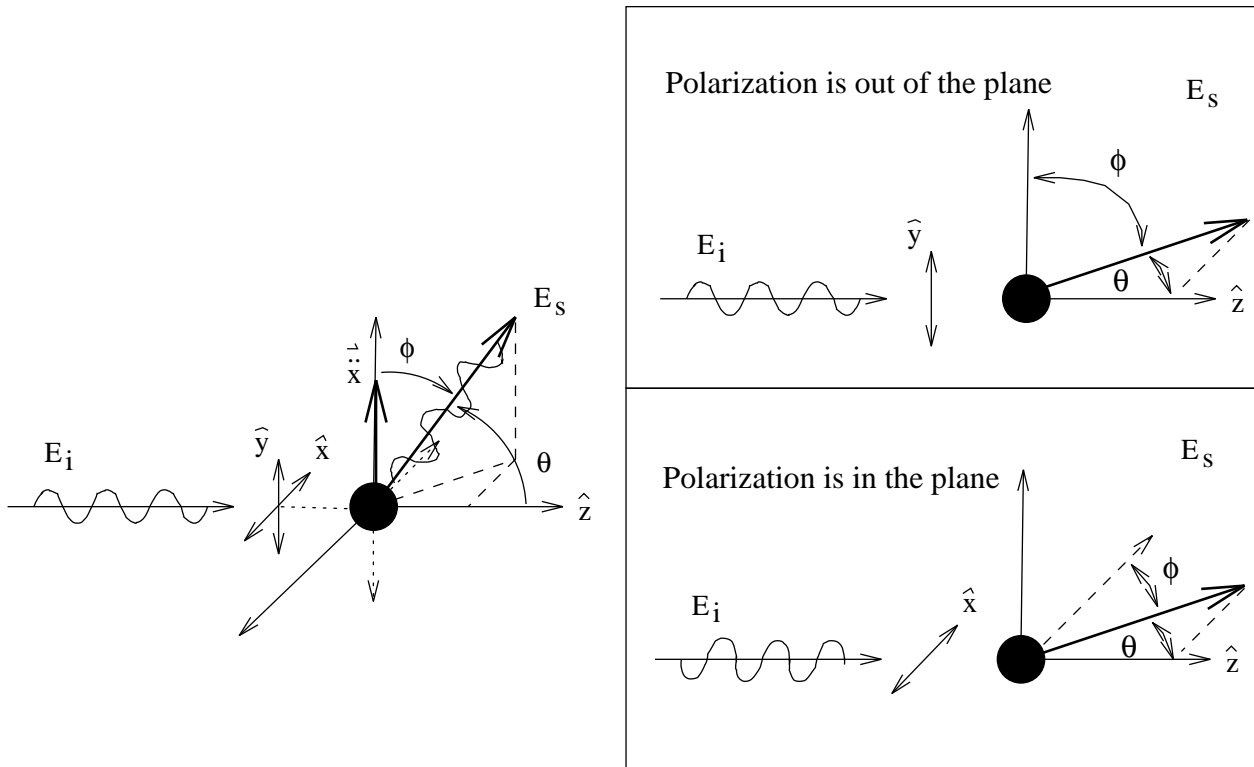
$$\ddot{\vec{x}} = \frac{e}{m}\vec{E} - \omega_0^2\vec{x}$$

Solution: $\vec{x} = x_0 e^{i\omega t} \hat{x}$ $x_0 = -\frac{eE_0}{m} \frac{1}{(\omega_0^2 - \omega^2)}$

$a = |\ddot{\vec{x}}| = \frac{\omega^2 eE_0}{m(\omega_0^2 - \omega^2)}$ Since $m_{nucleus} \gg m_{electron}$ No contribution by the nucleus.

The electron is accelerated in the x-direction and radiates energy. For exact details refer to any text on classical electrodynamics (e.g., Jackson, Reitz & Milford). Time and usefulness do not allow us to delve further.

There are however two components to the incident radiation:



(Assume that your eye /detector is in the x-z plane)

Note: ϕ is the angle between the scattered beam and the direction of the accelerated electron
 θ is the angle from the \hat{z} -axis

$$E_s = \frac{a e \sin\phi}{Rc^2} \quad \frac{E_s}{E_0} = -\frac{e^2 \omega^2 \sin\phi}{Rc^2 m(\omega_0^2 - \omega^2)}$$

$$\frac{I_s}{I_0} = \frac{E_s^2}{E_0^2} = +\frac{e^4 \omega^4 \sin^2\phi}{R^2 m^2 c^4 (\omega_0^2 - \omega^2)^2}$$

[Note: If $\omega \sim \omega_0$ (i.e., at an absorption edge) Thompson theory breaks down.]

In general, $\omega \gg \omega_0$ and the x-ray intensity $\propto \frac{1}{R^2}$ (a “light bulb”)

[Incoherent (i.e., Compton scattering) is also present.]

$$I_s = \frac{e^4}{R^2 m^2 c^4} \sin^2 \phi \quad I_0$$

As was just shown by viewing only in the x-z plane:

For x-rays polarized in the x-dir $\phi + \theta = \pi/2$

For x-rays polarized in the y-dir $\phi = \pi/2$

Thus for an unpolarized beam $I = \frac{1}{2}I_0(x - z) + \frac{1}{2}I_0(y - z)$

$$I_s = \left(\frac{e^2}{mc^2} \right)^2 \frac{1}{R^2} \frac{1}{2} \left[\sin^2 \pi/2 + \sin^2(\pi/2 - \theta) \right]$$

$$I_s = \frac{1}{R^2} \left(\frac{e^2}{mc^2} \right)^2 \frac{1 + \cos^2 \theta}{2} \quad \text{Polarization factor}$$

The polarization factor is just one of many necessary “corrections.”

Physics 0551 Lecture #3

Title: Scattering Due to Atoms

Last time we calculated the scattering of photons (using unpolarized incident radiation) from a single classically bound electron.

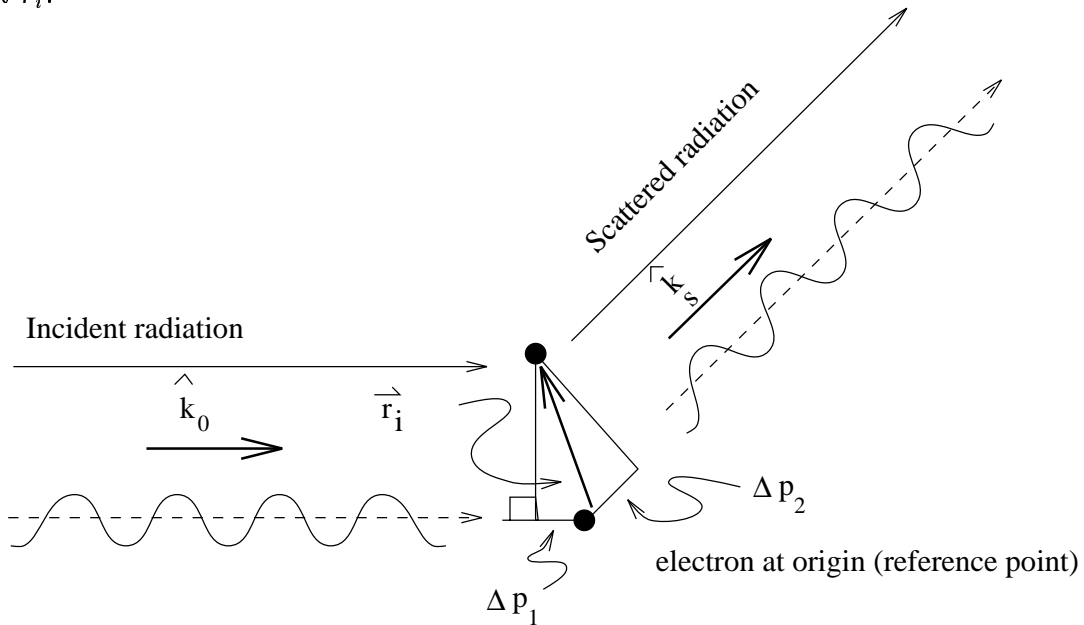
$$\frac{I_s}{I_o} = \frac{1}{R^2} \cdot \left(\frac{e^2}{mc^2} \right)^2 \frac{1 + \cos^2 \theta}{2}$$

Thus the total scattering cross section is given by:

$$\sigma_T = \int \int \frac{I_s}{I_o} R^2 \sin \theta d\theta d\phi = \frac{8}{3} \pi \left(\frac{e^2}{mc^2} \right)^2 = 0.67 \times 10^{-24} \text{ cm}^2.$$

In reality atoms are a collection of electrons. These electrons are spatially separated and to first order non-interacting. Thus, their scattering will not superimpose completely coherently.

For example, assume two electrons such that one is at the origin whilst the other is located at \vec{r}_i .



The incoming wave is described by

$$\vec{E}_i = \vec{E}_0 \exp \{ i(\omega_0 t - \vec{k}_0 \cdot \vec{r}) \}$$

and the outgoing wave is given by

$$\vec{E}_f = \vec{E}_s \exp \left\{ i(\omega_s t - \vec{k}_s \cdot \vec{r}) \right\}$$

Recall $\epsilon_{photon} = \hbar\omega = \hbar|k|c$, $\lambda = \frac{2\pi}{|k|}$, $\nu\lambda = c$

Since each electron independently scatters the incoming photon field, there is necessarily a path difference $\Delta p_1 + \Delta p_2$ between the scattered waves. This path difference implies a phase difference.

$$\Delta p_1 = -\hat{k}_0 \cdot \vec{r}_i$$

$$\Delta p_2 = +\hat{k}_s \cdot \vec{r}_i$$

$$\Delta p \equiv \Delta p_1 + \Delta p_2 = (\hat{k}_s - \hat{k}_0) \cdot \vec{r}_i \quad \Delta\phi \equiv \text{phase difference}$$

Assume **elastic** scattering $\lambda_0 = \lambda_s$ so

$$\Delta \text{path} \cdot \frac{2\pi}{\lambda} = \Delta\phi$$

$$\underline{\Delta\phi = (\vec{k}_s - \vec{k}_0) \cdot \vec{r}_i = \vec{s} \cdot \vec{r}_i}$$

and $\vec{k}_s - \vec{k}_0$ is the change in the “momentum” of the scattered waves (i.e., diffraction vector).

Thus we have a new and important quantity called the scattering vector or diffraction vector.

$$\vec{s} \equiv \vec{k}_d \equiv \vec{k}_s - \vec{k}_0$$

To get the total scattered amplitude for a single atom, it is clearly necessary to take the superposition of scattering from all the electrons.

The amplitude for the i^{th} electron is $A_i = f_e \exp i(\vec{s} \cdot \vec{r}_i)$ where f_e is the amplitude for an electron at the origin. Thus, the total amplitude is

$$A = \sum_{i=1}^Z A_i = f_e \sum_i \exp i(\vec{s} \cdot \vec{r}_i)$$

where Z is the atomic number.

$$I \equiv \text{intensity} = A^* A = f_e^2 \sum_j e^{-i\vec{s} \cdot \vec{r}_j} \sum_i e^{i\vec{s} \cdot \vec{r}_i}$$

$$I = f_e^2 \sum_{i,j} e^{i\vec{s} \cdot (\vec{r}_i - \vec{r}_j)}$$

This summation is for the superposition of point-like e^- 's. This distribution clearly changes with time. In actuality, the **time** averaged distribution is required. Replacing the point-like e^- 's with a charge distribution gives

$$A = f_e \int_V \rho(r) e^{i\vec{s} \cdot \vec{r}} dV$$

Thus a new quantity, $f_{\text{atom}} \equiv \frac{A}{f_e} \equiv$ Atomic scattering form factor, is realized.

Notice that as $\vec{s} \rightarrow 0$, (towards the forward scattering direction) the phase differences go to zero. Thus, intuitively one expects a smoothly decreasing intensity with increasing angle.

Now for the scattering from an arbitrary collection of atoms

$$A_T = \sum_{\text{atoms}}^{\text{all}} A_{\text{atom}} = \sum_k^{\text{atoms}} f_k e^{i\vec{s} \cdot \vec{r}_k}$$

where $f_k = f_e \int \rho_k(r) e^{i(\vec{s} \cdot \vec{r})} d\vec{r}$ for each atom

$\vec{r}_k \equiv$ position of the k^{th} atom $f_k \equiv$ atomic form factor for the k^{th} atom

The total observed intensity is

$$I_T = A_T^* A_T = \sum_{k,\ell} f_k f_\ell^* e^{i\vec{s} \cdot (\vec{r}_k - \vec{r}_\ell)}$$

Notice that at no point has the assumed periodicity of a crystalline lattice centered into this discussion! This will be done next time.

However, we will go a bit further.

ASSUME a collection of identical atoms:

$$I_T = \left(\sum_{k=\ell} + \sum_{k \neq \ell} \right) f_k f_\ell^* e^{i\vec{s} \cdot (\vec{r}_k - \vec{r}_\ell)}$$

$$I_T = \sum_{k=\ell} f_k f_k^* e^{i\vec{s} \cdot (\vec{r}_k - \vec{r}_k)} + \sum_{k \neq \ell} f_k f_\ell^* e^{i\vec{s} \cdot (\vec{r}_k - \vec{r}_\ell)}$$

Assume there are N *identical* atoms

$$I_T = N f^2 + \sum_{k \neq \ell} f_k f_\ell^* e^{i\vec{s} \cdot (\vec{r}_k - \vec{r}_\ell)} \quad (1)$$

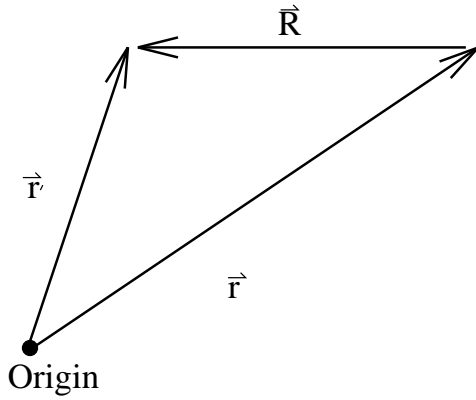
The first term has no phase or angular dependence. It represents a coherent background and is called the self-scattering term.

Another venture: Assume we replace the discrete sum of A_T with an atomic distribution function:

$$A_T(\vec{s}) = f \int_V \rho(\vec{r}) e^{i\vec{s} \cdot \vec{r}} dV$$

where f is the individual atom form factor and $\rho(\vec{r})$ is the atomic number density. Then

$$I(\vec{s}) = A(\vec{s}) A^*(\vec{s}) = |f|^2 \int \rho(\vec{r}) \rho(\vec{r}') e^{i\vec{s} \cdot (\vec{r} - \vec{r}')} d\vec{r} d\vec{r}'$$



$$\text{Let } \vec{r}' = \vec{r} + \vec{R}$$

Then the second term in Eqn. 1 (on the previous page) becomes

$$I'(s) = |f|^2 \int \int \rho(\vec{r}) \rho(\vec{r} + \vec{R}) e^{i\vec{s} \cdot \vec{R}} d\vec{r} d(\vec{r} + \vec{R})$$

We can define a new quantity

$$P(\vec{R}) \equiv \int \rho(\vec{r}) \rho(\vec{r} + \vec{R}) d\vec{r} \equiv \text{pair distribution function}$$

Now

$$I'(\vec{s}) = |f|^2 \int \rho(\vec{R}) e^{i\vec{s} \cdot \vec{R}} d\vec{R}$$

Clearly, $I'(\vec{s})$ is just the Fourier transform of the pair distribution function.

IMPORTANT - This quantity is what a diffraction experiment **extracts**

From this information and insight the actual atomic positions can often be ascertained.

Physics 0551 Lecture #4

Title: Coherent Scattering from a crystal.

Scattering from a periodic arrangement of atoms and the construction of the reciprocal lattice.

Recall the total atomic scattering amplitude

$$A(\vec{s}) = \sum_k^{\text{all atoms}} f_k e^{i\vec{s}\cdot\vec{r}_k}$$

Now invoke lattice periodicity

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

And also assume (at present) there is just one atom per unit cell

$$\vec{r}_k = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3 \quad f_k = f$$

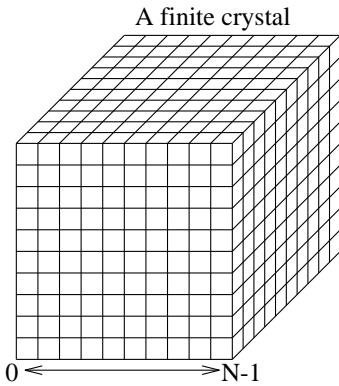
Thus

$$A(\vec{s}) = f \sum_k^{\text{all atoms}} e^{i\vec{s}\cdot(n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3)}$$

This sum is somewhat awkward to follow if $n_1, n_2, n_3 \rightarrow \infty$. Let us examine the sum in the range $0 \leq n_1, n_2, n_3 \leq N-1$. Hence there are only N^3 atoms to deal with.

$$A(\vec{s}) = f \sum_{n_1=0}^{N-1} e^{i(\vec{s}\cdot\vec{a}_1)n_1} \sum_{n_2=0}^{N-1} e^{i(\vec{s}\cdot\vec{a}_2)n_2} \sum_{n_3=0}^{N-1} e^{i(\vec{s}\cdot\vec{a}_3)n_3}$$

Now each sum can be simplified if the following substitution is made:



$$\begin{aligned} \sum_{n=0}^{N-1} e^{i(\vec{s}\cdot\vec{a})n} &= \sum_{n=0}^{\infty} e^{i(\vec{s}\cdot\vec{a})n} - \sum_{n=N}^{\infty} e^{i(\vec{s}\cdot\vec{a})n} \\ &= \sum_{n=0}^{\infty} e^{i(\vec{s}\cdot\vec{a})n} - e^{i(\vec{s}\cdot\vec{a})N} \sum_{n=0}^{\infty} e^{i(\vec{s}\cdot\vec{a})n} \\ &= (1 - e^{iN(\vec{s}\cdot\vec{a})}) \sum_{n=0}^{\infty} e^{i(\vec{s}\cdot\vec{a})n} \\ &= (1 - e^{iN(\vec{s}\cdot\vec{a})}) \frac{1}{1 - e^{i(\vec{s}\cdot\vec{a})}} \frac{1 - e^{-i(\vec{s}\cdot\vec{a})}}{1 - e^{i(\vec{s}\cdot\vec{a})}} \\ &= \frac{(1 - e^{iN(\vec{s}\cdot\vec{a})}) (1 - e^{-i(\vec{s}\cdot\vec{a})})}{2(1 - \cos \vec{s}\cdot\vec{a})} \end{aligned}$$

or

$$A(\vec{s}) = \frac{f \left[1 - e^{iN(\vec{s}\cdot\vec{a}_1)} \right] \left[1 - e^{iN(\vec{s}\cdot\vec{a}_2)} \right] \left[1 - e^{iN(\vec{s}\cdot\vec{a}_3)} \right] \left(1 - e^{-i\vec{s}\cdot\vec{a}_2} \right) \left(1 - e^{-i\vec{s}\cdot\vec{a}_3} \right) \left(1 - e^{-\vec{s}\cdot\vec{a}_3} \right)}{2(1 - \cos \vec{s}\cdot\vec{a}_1) 2(1 - \cos \vec{s}\cdot\vec{a}_2) 2(1 - \cos \vec{s}\cdot\vec{a}_3)}$$

The intensity $I = A^*A$ gives

$$I = |f|^2 \frac{(1 - \cos N \vec{s}\cdot\vec{a}_1)(1 - \cos \vec{s}\cdot\vec{a}_1) \dots (1 - \cos N \vec{s}\cdot\vec{a}_3)(1 - \cos \vec{s}\cdot\vec{a}_3)}{(1 - \cos \vec{s}\cdot\vec{a}_1)^2 \dots (1 - \cos \vec{s}\cdot\vec{a}_3)^2}$$

$$I = |f|^2 \frac{(1 - \cos N \vec{s}\cdot\vec{a}_1)(1 - \cos N(\vec{s}\cdot\vec{a}_2)) (1 - \cos N(\vec{s}\cdot\vec{a}_3))}{(1 - \cos \vec{s}\cdot\vec{a}_1)(1 - \cos \vec{s}\cdot\vec{a}_2)(1 - \cos \vec{s}\cdot\vec{a}_3)}$$

or

$$I = |f|^2 \frac{\sin^2(N(\vec{s}\cdot\vec{a}_1)/2)\sin^2(N\vec{s}\cdot\vec{a}_2/2)\sin^2(N\vec{s}\cdot\vec{a}_3/2)}{\sin^2(\vec{s}\cdot\vec{a}_1/2)\sin^2(\vec{s}\cdot\vec{a}_2/2)\sin^2(\vec{s}\cdot\vec{a}_3/2)}$$

The behavior of the intensity is relatively straightforward. Let $N=10$ and let both $\vec{s}\cdot\vec{a}_2 = 2\pi n$ and $\vec{s}\cdot\vec{a}_3 = 2\pi m$. Thus (for one set of terms)

$$\frac{\sin^2 N\vec{s}\cdot\vec{a}_2/2}{\sin^2 \vec{s}\cdot\vec{a}_2/2} = \frac{\sin^2 N\pi n}{\sin^2 \pi n} = N^2 \text{ (using L'Hopital's rule)}$$

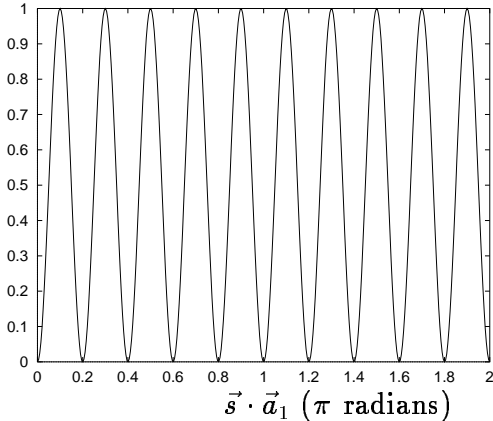
or since $\sin(N\pi n) \rightarrow 0$ expand top and bottom in Taylor's series $\sin x \sim x$ if $x \rightarrow 0$ (choose $n = 0$)

$$\frac{\sin^2 N\pi n}{\sin^2 \pi n} \sim \frac{(N\pi n)^2}{(\pi n)^2} = N^2$$

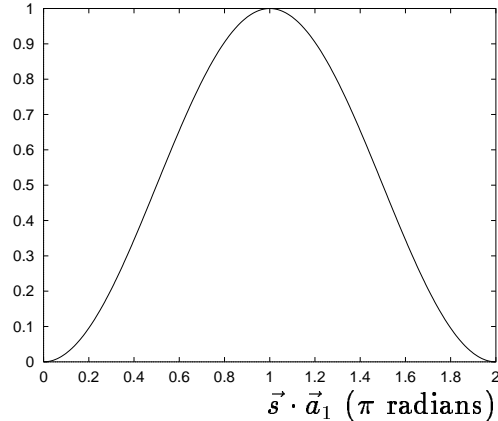
Thus

$$I = |f|^2 \frac{\sin^2 N \vec{s}\cdot\vec{a}_1}{\sin^2 \vec{s}\cdot\vec{a}_1} N^4$$

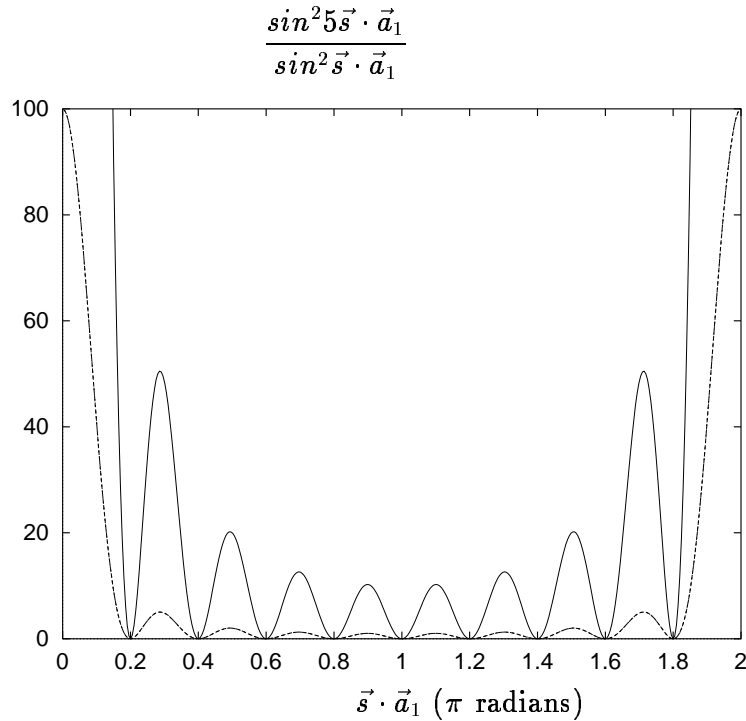
Plot: Numerator = $\sin^2 5(\vec{s}\cdot\vec{a}_1)$ and



Denominator = $\sin^2(\vec{s}\cdot\vec{a}_1)$ ($0 \leq \vec{s}\cdot\vec{a}_1 \leq 2\pi$)



Now for

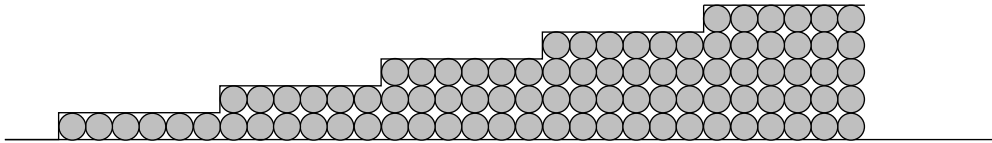


So

$$I(0) = |f|^2 10^2 10^2 10^2 = |f|^2 N^6$$

Now compare this intensity with the self scattering which was proportional to the number of atoms or N^3 (in this case) when $N^3 \sim 10^{23}$ atoms!

In addition, as N becomes large the intensity due to finite size effects (so called “F” peaks) become unobservable. However, these fringes can be seen in very small crystals using electron diffraction. They can also be seen in surface scattering from crystals with steps.



As $N \rightarrow \infty$, the curves become δ -functions with FWHM (Full widths at half maximum) of $2\pi/N$ and height N^6 at the positions

$$\left. \begin{aligned} \vec{s} \cdot \vec{a}_1 &= 2\pi h \\ \vec{s} \cdot \vec{a}_2 &= 2\pi k \\ \vec{s} \cdot \vec{a}_3 &= 2\pi \ell \end{aligned} \right\} \begin{array}{l} h, k, \ell \text{ are integers} \\ \text{This is the Laue condition!} \end{array}$$

This set of expressions are called the Laue diffraction conditions. When $\vec{s} \cdot \vec{a}_1$, $\vec{s} \cdot \vec{a}_2$, $\vec{s} \cdot \vec{a}_3$ are all multiples of 2π , the amplitudes interfere constructively. This condition is equivalent to Bragg’s law $n\lambda = 2d \sin\theta$. (Constructive interference a scattered waves)

To review:

One atom per unit with a crystal length of $N-1$ on a side

$$A(\vec{s}) = f \sum_i^{N^3 \text{ sites}} e^{i\vec{s} \cdot (n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3)}$$

gives

$$I = |f|^2 \frac{\sin^2(N\vec{s} \cdot \vec{a}_1)/2 \dots}{\sin^2(\vec{s} \cdot \vec{a}_1)/2 \dots}$$

If we *restrict* our sum to \vec{s} 's such that the Laue conditions are met then $\vec{s} \cdot \vec{a}_i = 2\pi\ell$ and all of the scattering is coherent. ($i = 1, 2, 3$)

$$A(\vec{s}) = fN^3$$

If we define a normalizing $f = f'/N^3$, then

$$A(\vec{s}) = f' \text{ (N independent)}$$

What if there are two atoms per cell

Atom A is located at $n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3$

While Atom B is at $n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3 + \vec{\Delta}$ where $\vec{\Delta}$ is *not* a lattice vector.

$$\text{The total } A(\vec{s}) = f_A \sum_j^{N^3 \text{ sites}} e^{i\vec{s} \cdot (n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3)} + f_B \sum_j^{N^3 \text{ sites}} e^{i\vec{s} \cdot (n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3 + \vec{\Delta})}$$

Restrict sum to those that satisfy the Laue condition. The set of \vec{s} 's which satisfy the Laue condition are designated \vec{G} and are called the *reciprocal lattice vectors*.

$$A(\vec{G}) = f_A N^3 + f_B N^3 e^{i\vec{G} \cdot \vec{\Delta}} \quad f' = f/N^3$$

$$A(\vec{G}) = f'_A + f'_B e^{i\vec{G} \cdot \vec{\Delta}} \rightarrow \text{there are two terms here, one for each atom within the unit cell (the basis).}$$

Generalizing gives

$$A(\vec{G}) = \sum_j^{\substack{\text{unit cell} \\ \text{atoms}}} f_j e^{i\vec{G} \cdot \vec{r}_j} \text{ and } I(\vec{G}) = A * A \equiv \text{structure factor}$$

\vec{r}_j is the relative position of atoms within the unit cell.