Chapter 2

Wave Diffraction and the Reciprocal Lattice

PHYS 432

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Chapter Topics

1. Wave Diffraction by Crystals
2. Bragg Law
3. Scattered Wave Amplitude
4. Brillouin Zones
5. Reciprocal Lattice
6. Fourier Analysis of the Basis

Incident light on the CD is white. Why so many separate colors can be seen on the CD instead of a reflection of only white light?

The tracks of a compact disc act as a diffraction grating, producing a separation of the colors of white light. The nominal track separation on a CD is 1.6 micrometers, corresponding to about 625 tracks per millimeter. This is in the range of ordinary laboratory diffraction gratings. For red light of wavelength 600 nm, this would give a first order diffraction maximum at about 22° .

http://hyperphysics.phy-astr.gsu.edu/hbase/phyopt/grating.html

Diffraction of Waves by Crystalline Solids

- We know that a crystal is a periodic structure with unit cells that are repeated regularly.

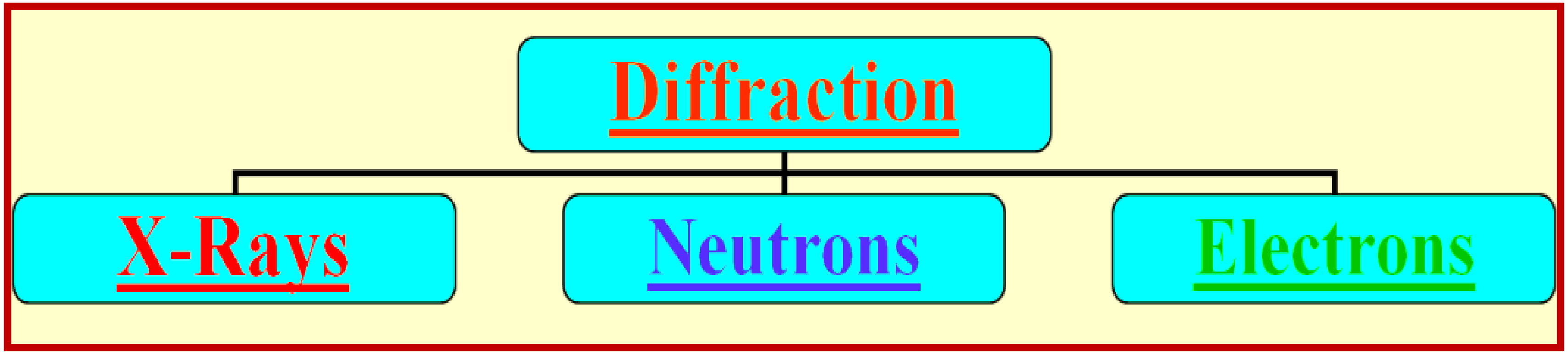
- ***Crystal Structure Information*** can be obtained by understanding **the diffraction patterns of waves** (of appropriate wavelengths) ***interacting with the solid*****.**

- Analysis of such diffraction patterns is the main topic of this chapter.

- Diffraction patterns are produced by constructive and destructive interferences of waves.

Diffraction of Waves by Crystalline Solids

- It is common to study crystal structures by **X-ray, Neutron, and Electron diffraction**. The general principles of diffraction are same for all waves.



Diffraction

X-Rays

Neutrons

Electrons

- The results of crystal diffraction depend on the crystal structure and on the wavelength.

- **At optical wavelengths** such as **5,000 Å**, the superposition of waves scattered elastically by the individual atoms of a crystal ***results in ordinary optical reflection and refraction***.

- When **the wavelength** of radiation is ***comparable to or smaller than the lattice constant***, diffracted beams produce diffraction pattern.

Wavelength vs Energy

Quantum Mechanical Result

- The energy & momentum of a particle with **De Broglie Wavelength λ** are

$$E = (hc/\lambda) \quad \& \quad p = (h/\lambda)$$

(**h = Planck's constant**)

- Diffraction from crystal planes requires that λ be of the same order of magnitude as the **distance d** between planes:

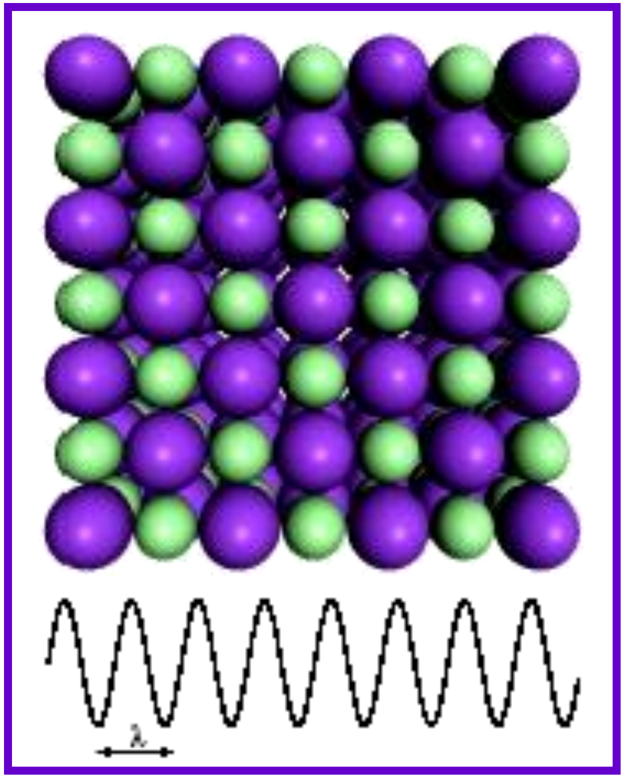
$$d \approx \text{a few Angstroms (Å)}$$

- So λ must also be a few Angstroms (Å).

X-Ray Crystallography

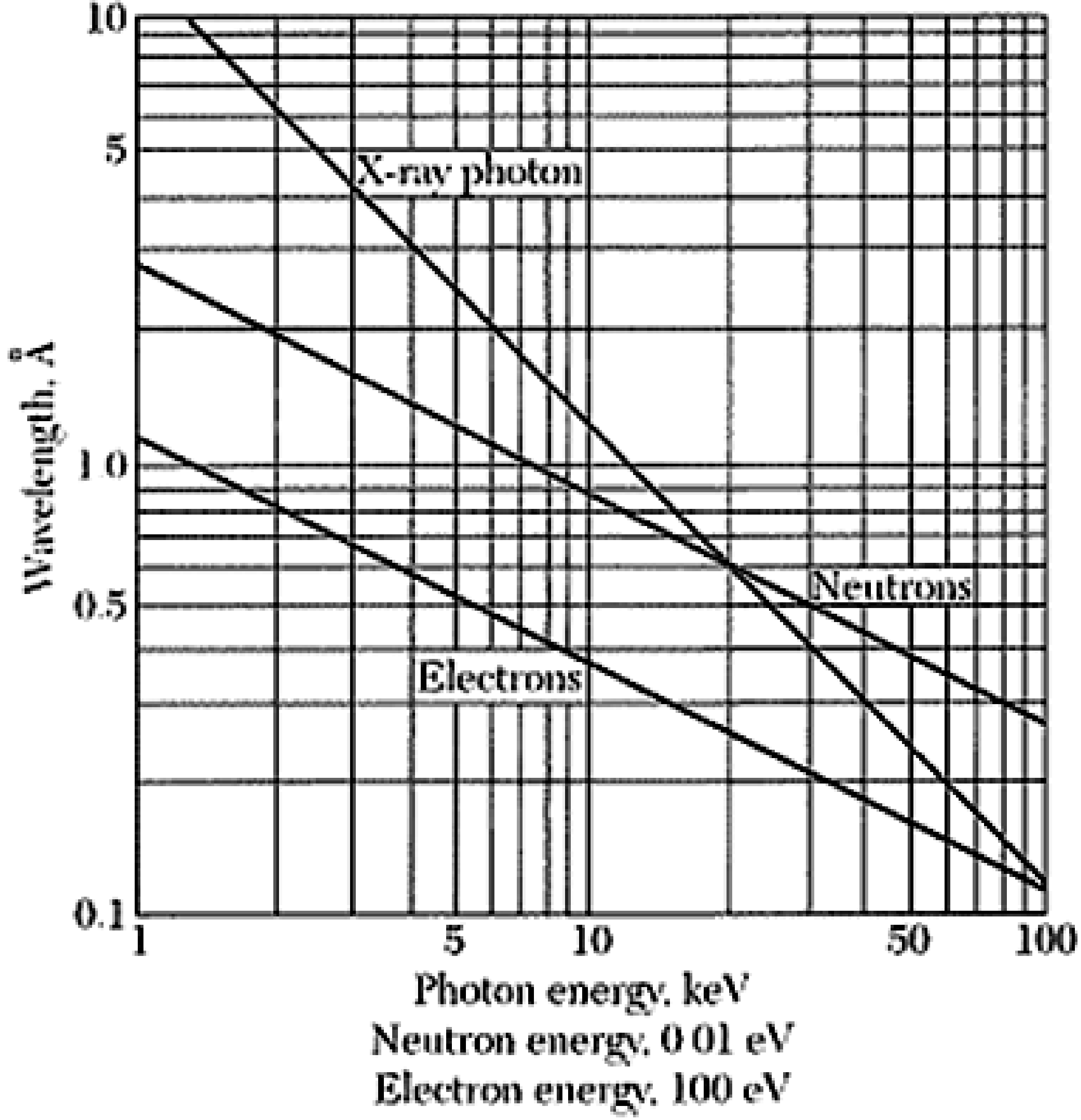
- For **X-Rays**, the wavelength **λ** is typically **≈ a few Ångstroms**, which is comparable to the interatomic spacing (distance between atoms or ions) in crystals.

- For crystal structure determination, the **X-Rays** have to be of energy:

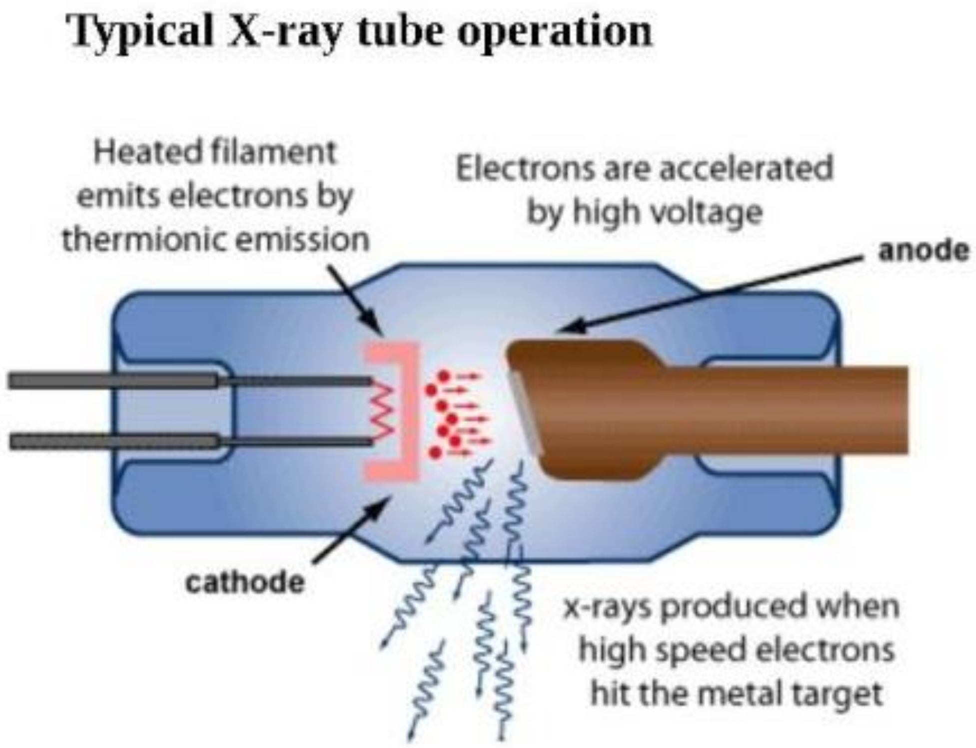


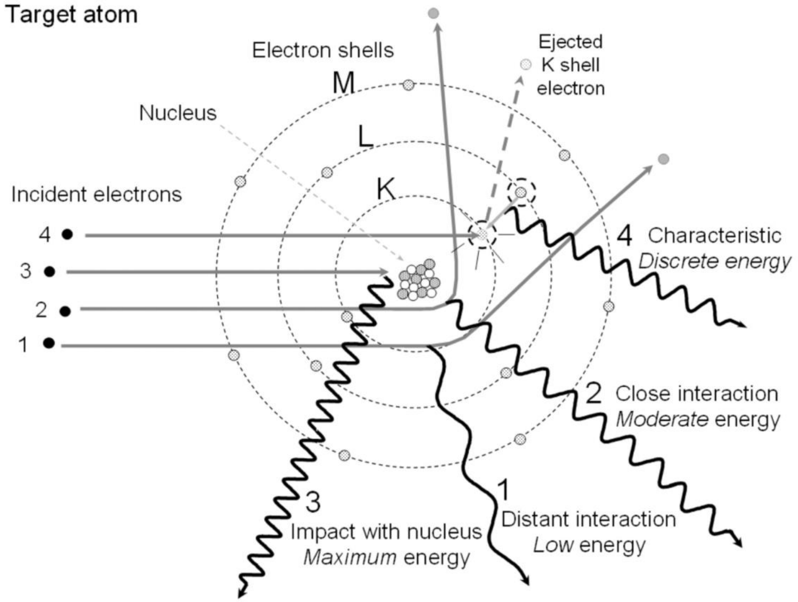
$$E_{x-ray} = \hbar\omega = h\upsilon = \frac{hc}{\lambda} = \frac{hc}{1x10^{-10}m} = 12.3x10^{3}eV$$

Wavelength vs Energy



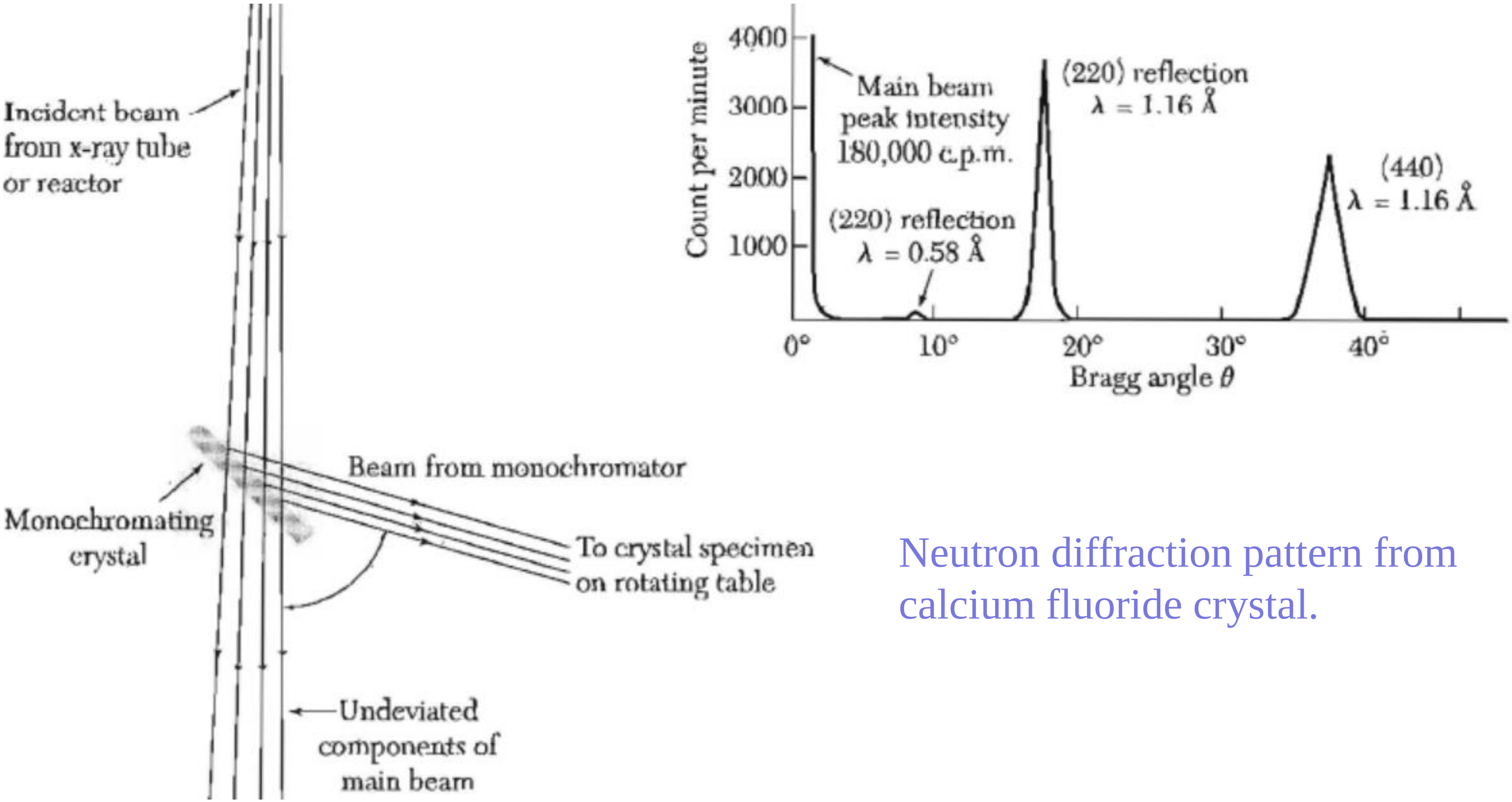
How X-rays are produced?





https://tech.snmjournals.org/content/32/3/139.figures-only
https://www.designworldonline.com/x-rays-and-ionizing-radiation/

Monochromator and Neutron Diffraction



Neutron diffraction pattern from calcium fluoride crystal.

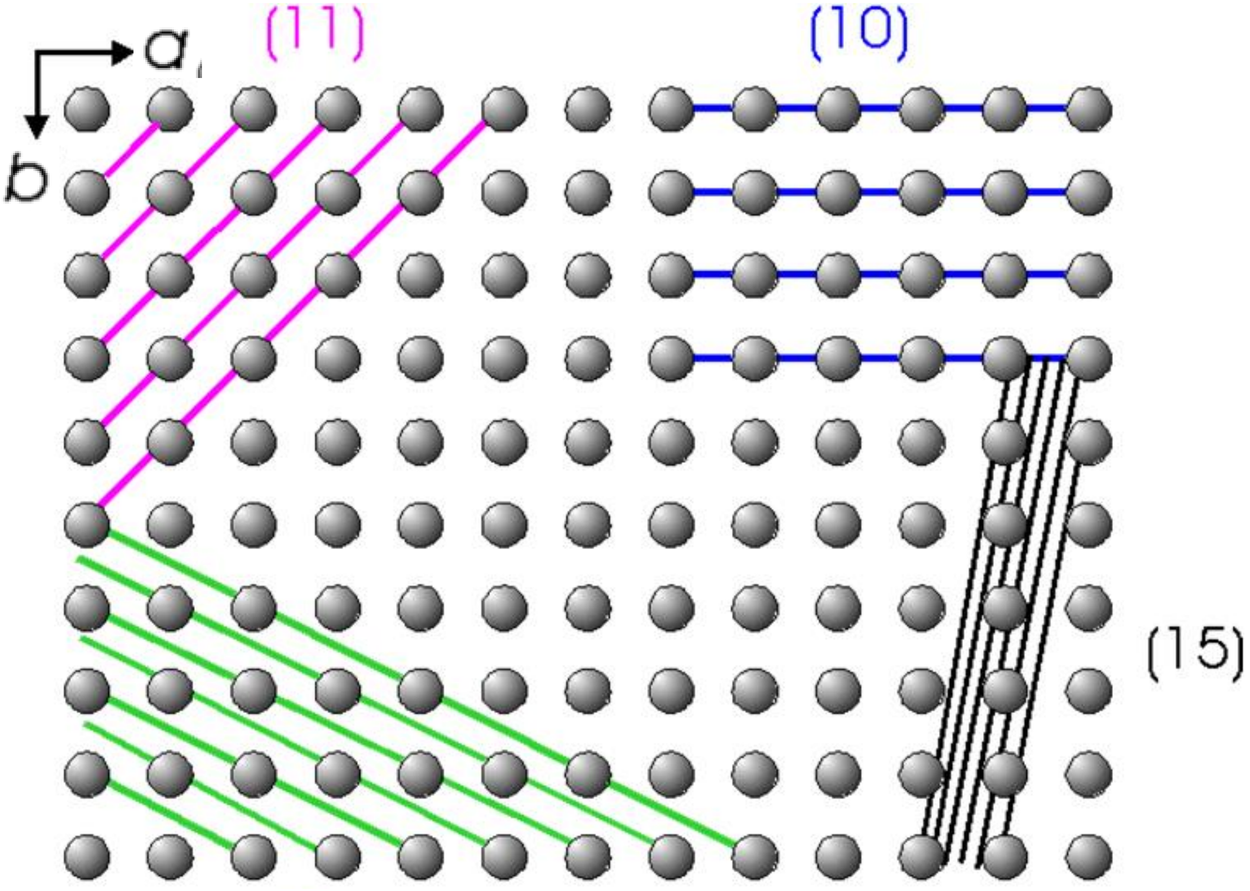
Monochromator selects a narrow spectrum of x-ray or neutron wavelengths from a broad spectrum of incident beam.

X-Ray Diffraction of Crystals

- Beam diffraction takes place ***only in certain specific directions*** (certain angles of incidence θ), much as light is diffracted by a grating.

- By measuring the ***directions of the diffraction*** and the ***angles corresponding to intensities due to constructive interference***, information about the ***Crystal Structure*** such as lattice constant, crystal structure etc. can be obtained.

Meaning of *d* for 2D

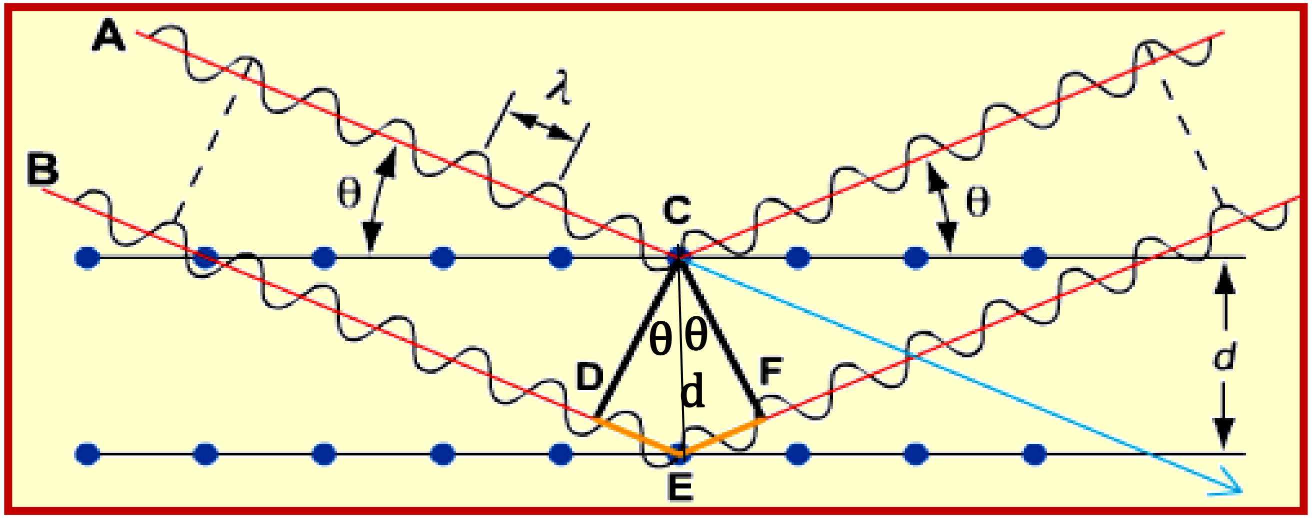


$(\bar{2}1)$

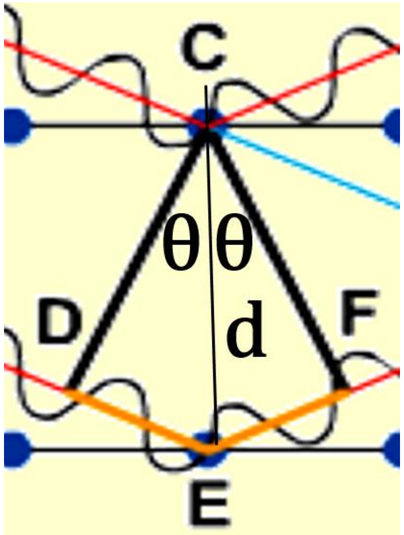
Bragg Law

- Incident waves are reflected specularly from parallel planes of atoms in the crystal, with each plane reflecting only a very small fraction of the radiation, like a lightly silvered mirror.

- In specular (mirrorlike) reflection, the angle of incidence is equal to the angle of reflection.



Bragg Law



- The length DE is the same as EF, so the total distance traveled by the bottom wave is expressed by:
- *Constructive interference* of the radiation from successive planes occurs when the path difference is an integral number of wavelengths. Note that line **CE = d =** distance between the 2 layers.

$$\boxed{EF = d\sin\theta} \qquad \boxed{DE = d\sin\theta}$$

$$\boxed{DE + EF = 2d\sin\theta}$$

For constructive interference, the path difference should be integral multiple of wavelength.

$$\boxed{n\lambda = 2d\sin\theta}$$

This is called the ***Bragg Law.***

$$\boxed{2d \sin\theta = n\lambda}$$

d = Spacing between the Planes, n = Order of Diffraction.

- Because **$\sin\theta \leq 1$**,

***Bragg reflection can only occur for wavelengths satisfying*:** $\boxed{n\lambda \leq 2d}$

- This is why visible light can't be used for studying crystal structures.

- The Bragg derivation is simple but it is convincing, since only it reproduces the result that agrees with observations.

- Diffracted beams (reflections) from any set of lattice planes can only occur at particular angles predicted by **Bragg's Law**.

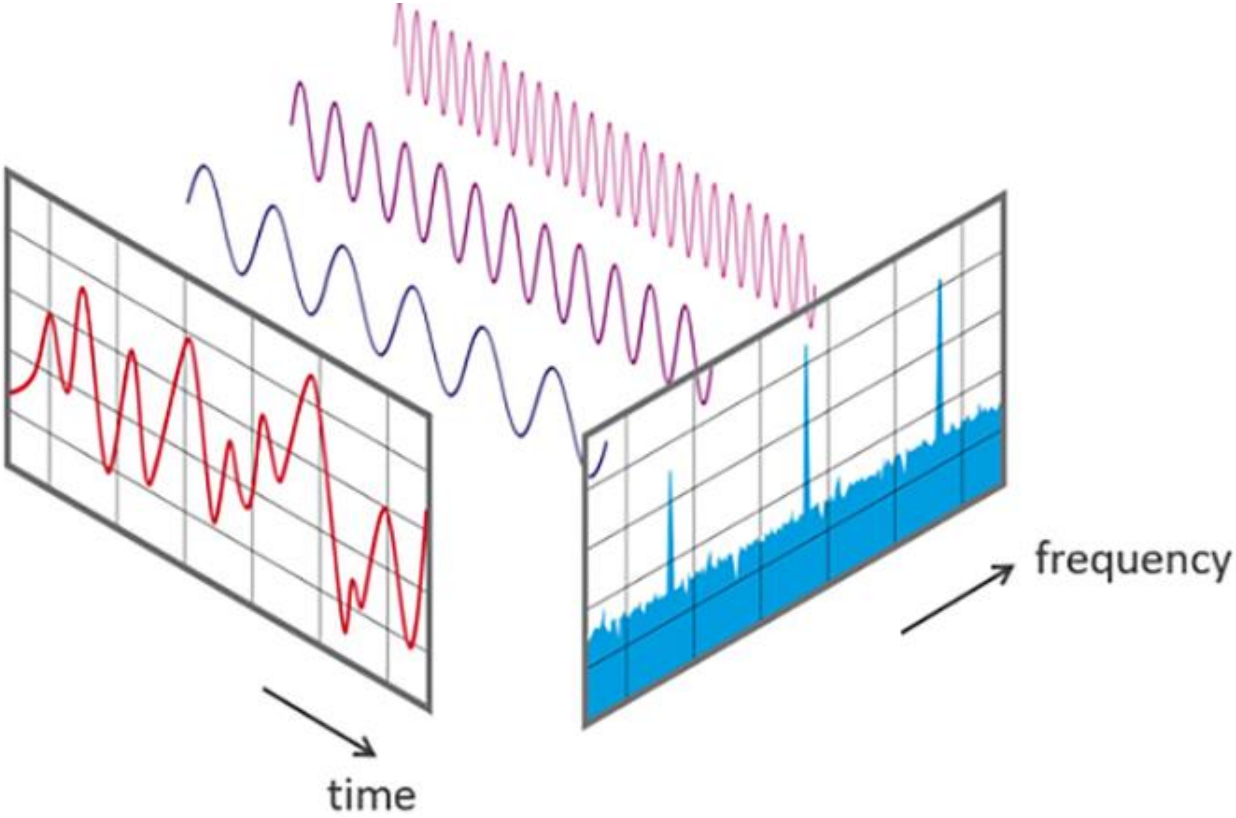
Bragg Reflections

- Although the reflection from each plane is specular, ***only for certain values of θ will the reflections from all planes add up in phase to give a strong reflected beam.***
- Each plane reflects only **10^{-3} to 10^{-5}** of the incident radiation, i.e. it is not a perfect reflector.
- **So, 10^3 to 10^5 planes contribute to the formation of the Bragg-reflected beam in a perfect crystal.**
- The composition of the basis determines the relative intensity of the various orders of diffraction.

- **Scattered Wave Amplitude**
- **Diffraction Condition in the Reciprocal Lattice**
- **Brillouin Zones**

- What is meant by Fourier analysis?

- The process of decomposing a function into oscillatory components is called Fourier analysis, i.e. any general function may be represented or approximated by sums of simpler trigonometric functions.



Scattered Wave Amplitude

- The Bragg law gives the condition for the constructive interference of waves scattered from lattice planes.
- Deeper analyses are needed to determine the scattering intensity from the basis of atoms, i.e. scattering due to the spatial distribution of electrons within each cell.
- Periodicity of the electron number density n(r) will be used for performing Fourier analysis.
- Fourier analysis give a second lattice (reciprocal lattice) associated with the direct crystal.

Scattered Wave Amplitude

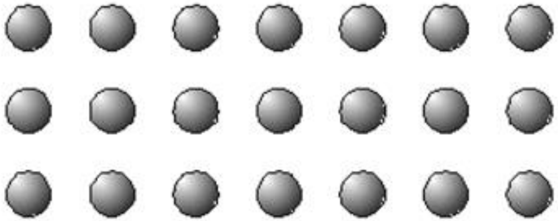
Any local physical property of the crystal, such as the charge concentration, electron number density, or magnetic moment density is invariant under translation by a vector T. The vector **T** is the

Direct Lattice Translation Vector:

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

The electron number density **n(r)** in the crystal is a periodic function in space:

$$n(\mathbf{r}) = n(\mathbf{r} + \mathbf{T})$$



Periodic Functions and Fourier Analysis

- Any periodic function can be expressed in terms of its periodic Fourier components (harmonics).

- For example electron number density n(x) is a periodic function of $\boldsymbol{x}$, with period $\boldsymbol{a}$ in 1D crystal and is invariant under translation $\mathbf{T}$, such that:

$$n(\mathbf{x} + \mathbf{T}) = n(\mathbf{x})$$

- Such periodicity creates an ideal situation for Fourier analysis.

Periodic Functions and Fourier Analysis

- If we expand n(x) in Fourier of sines and cosines we get:

$$n(x) = n_0 + \sum_{p>0} \left[C_p \cos(2\pi px/a) + S_p \sin(2\pi px/a) \right] = \sum_p n_p e^{i2\pi px/a}$$

- The **p's** are integers.
- The Fourier coefficient of the number density can be written:

$$n_p = \frac{1}{a} \int_0^a dx n(x) e^{-i2\pi px/a}$$

Periodic Functions and Fourier Analysis

$$n(x) = \Sigma_p\, n_p\, e^{i2\pi px/a}$$

The factor $2\pi/a$ in the argument ensures that n(x) has the period a:

$$n(x+a) = n_0 + \Sigma_{p>0}[C_p \cos(2\pi\, p\, x/a + 2\,\pi p) + S_p \sin(2\pi\, p\, x/a + 2\,\pi p)\,]$$
$$= n_0 + \Sigma_{p>0}[C_p \cos(2\pi\, p\, x/a) + S_p \sin(2\pi\, p\, x/a)\,] = n(x)$$

We can say that $2\pi\, p/a$ is a point in the reciprocal lattice or Fourier space of the crystal.

The extension of the Fourier analysis to periodic function in 3D can be written as:

$$n(\mathbf{r}) = \Sigma_G\, n_G \exp(i\, \mathbf{G}.\mathbf{r})$$

Periodic functions and Fourier Analysis

$$n(r) = \Sigma_G\, n_G\, e^{i\,\mathbf{G}\cdot\mathbf{r}}$$

where the **G**'s are vectors, i.e.,

$$e^{i\,\mathbf{G}\cdot\mathbf{r}} = e^{i\,(G_x x + G_y y + G_z z)}$$

A periodic function satisfies

$$n(\boldsymbol{r}+\boldsymbol{T}) = n(\boldsymbol{r})$$

where T is any translation

$$\boldsymbol{T}(n_1, n_2, n_3) = n_1\,\boldsymbol{a_1} + n_2\,\boldsymbol{a_2} + n_3\,\boldsymbol{a_3}\,;$$ where n's are integers

Thus

$$n(\mathbf{r}+\mathbf{T}) = \Sigma_G\, n_G\, e^{i\,\mathbf{G}\cdot(\mathbf{r}+\mathbf{T})} = \Sigma_G\, n_G\, e^{i\,\mathbf{G}\cdot\mathbf{r}}\, e^{i\,\mathbf{G}\cdot\mathbf{T}} = n(\,\mathbf{r}\,)$$

$$\Rightarrow e^{i\,\mathbf{G}\cdot\mathbf{T}} = 1 \Rightarrow \mathbf{G}\cdot\mathbf{T} = 2\pi \times \text{integer}$$

The vectors G are called *Reciprocal Lattice Vectors*

- Only ***the set of reciprocal lattice vectors*** **G** that satisfy $e^{i\,\boldsymbol{G}.\boldsymbol{T}} = 1$ lead to an electron number density **n(r)** that is invariant under lattice translations.
- It's not too hard to show that the set of **G's** that meet this requirement are of the form

$$\boxed{\mathbf{G} = v_1\mathbf{b}_1 + v_2\mathbf{b}_2 + v_3\mathbf{b}_3}$$

where $\boldsymbol{\upsilon}_1$, $\boldsymbol{\upsilon}_2$ & $\boldsymbol{\upsilon}_3$ are integers & the $\mathbf{b}_i$'s are reciprocal lattice vectors which are defined on the next page.

- Every crystal structure has two lattices associated with it, the crystal lattice and the reciprocal lattice.
- A diffraction pattern of a crystal is a map of the reciprocal lattice of the crystal.
- An atomically resolved image of crystal is a map of the crystal structure in real space.

$$\bar{b}_1 = 2\pi \frac{\bar{a}_2 \times \bar{a}_3}{\bar{a}_1 . \bar{a}_2 \times \bar{a}_3} \qquad \bar{b}_2 = 2\pi \frac{\bar{a}_3 \times \bar{a}_1}{\bar{a}_1 . \bar{a}_2 \times \bar{a}_3} \qquad \bar{b}_3 = 2\pi \frac{\bar{a}_1 \times \bar{a}_2}{\bar{a}_1 . \bar{a}_2 \times \bar{a}_3}$$

If a_1, a_2, a_3 are the primitive vectors of the crystal lattice then b_1, b_2, and b_3 are the primitive vectors of the reciprocal lattice.

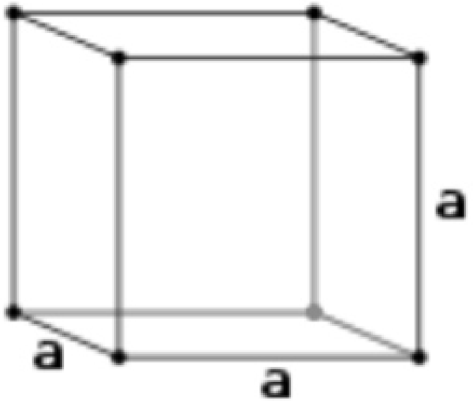
$$\boxed{\mathbf{b}_i = 2\pi \frac{\mathbf{a}_j \times \mathbf{a}_k}{\mathbf{a}_i \cdot \left(\mathbf{a}_j \times \mathbf{a}_k\right)}, \quad i = x, y, z \;\rightarrow\; \mathbf{b}_i \cdot \mathbf{a}_j = 2\pi\delta_{ij}}$$

where $\delta_{ii} = 1$, $\delta_{ij} = 0$ if $i \neq j$

If real lattice is Bravais lattice so is the reciprocal lattice.

Vectors in the direct lattice have dimension of ***[length]***, whereas the vectors in the reciprocal lattice have the dimensions of ***[1/length]***,

Reciprocal lattice vectors of SC



$$\mathbf{b}_i = 2\pi \frac{\mathbf{a}_j \times \mathbf{a}_k}{\mathbf{a}_i \cdot \left(\mathbf{a}_j \times \mathbf{a}_k\right)},\ i = x, y, z \rightarrow \mathbf{b}_i \cdot \mathbf{a}_j = 2\pi\delta_{ij}$$

$$\mathrm{V} = |\boldsymbol{b_1}.(\boldsymbol{b_2} \times \boldsymbol{b_3})|$$

	Direct Lattice	**Reciprocal Lattice**	**Volume**
SC	$\begin{cases} \mathbf{a}_1 = a\mathbf{x} \\ \mathbf{a}_2 = a\mathbf{y} \\ \mathbf{a}_3 = a\mathbf{z} \end{cases}$	$\begin{cases} \mathbf{b}_1 = (2\pi/a)\mathbf{x} \\ \mathbf{b}_2 = (2\pi/a)\mathbf{y} \\ \mathbf{b}_3 = (2\pi/a)\mathbf{z} \end{cases}$	$(2\pi/a)^3$

Reciprocal Lattices for the SC, FCC & BCC Lattices

Direct Lattice | **Reciprocal Lattice** | **Volume**

FCC

$$\begin{cases} \mathbf{a}_1 = \frac{1}{2}a(\mathbf{x}+\mathbf{y}) \\ \mathbf{a}_2 = \frac{1}{2}a(\mathbf{y}+\mathbf{z}) \\ \mathbf{a}_3 = \frac{1}{2}a(\mathbf{z}+\mathbf{x}) \end{cases} \qquad \begin{cases} \mathbf{b}_1 = \frac{2\pi}{a}(-\mathbf{x}+\mathbf{y}-\mathbf{z}) \\ \mathbf{b}_2 = \frac{2\pi}{a}(\mathbf{x}-\mathbf{y}+\mathbf{z}) \\ \mathbf{b}_3 = \frac{2\pi}{a}(\mathbf{x}+\mathbf{y}-\mathbf{z}) \end{cases} \qquad 2(2\pi/a)^3$$

BCC

$$\begin{cases} \mathbf{a}_1 = \frac{1}{2}a(\mathbf{x}+\mathbf{y}-\mathbf{z}) \\ \mathbf{a}_2 = \frac{1}{2}a(-\mathbf{x}+\mathbf{y}+\mathbf{z}) \\ \mathbf{a}_3 = \frac{1}{2}a(\mathbf{x}-\mathbf{y}+\mathbf{z}) \end{cases} \qquad \begin{cases} \mathbf{b}_1 = \frac{2\pi}{a}(\mathbf{y}+\mathbf{z}) \\ \mathbf{b}_2 = \frac{2\pi}{a}(\mathbf{x}+\mathbf{z}) \\ \mathbf{b}_3 = \frac{2\pi}{a}(\mathbf{x}+\mathbf{y}) \end{cases} \qquad 4(2\pi/a)^3$$

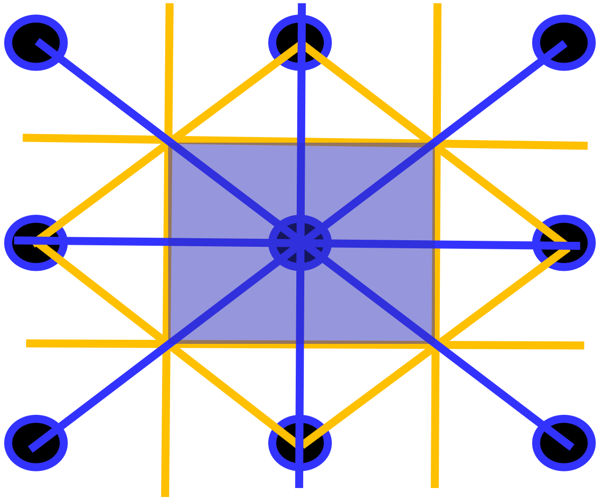
- **Brillouin Zones**

- **Diffraction Condition in the Reciprocal Lattice**

- **The reciprocal lattice consists of points in 3D. How would the lattice points transform in 2D?**

Brillouin Zones

The ***Brillouin Zone*** **(BZ)** is defined as ***the Wigner-Seitz primitive cell in the reciprocal lattice*****.** It gives a geometric interpretation, in the reciprocal lattice, of the diffraction condition.



- The Brillouin construction exhibits all wavevectors **k** that can be

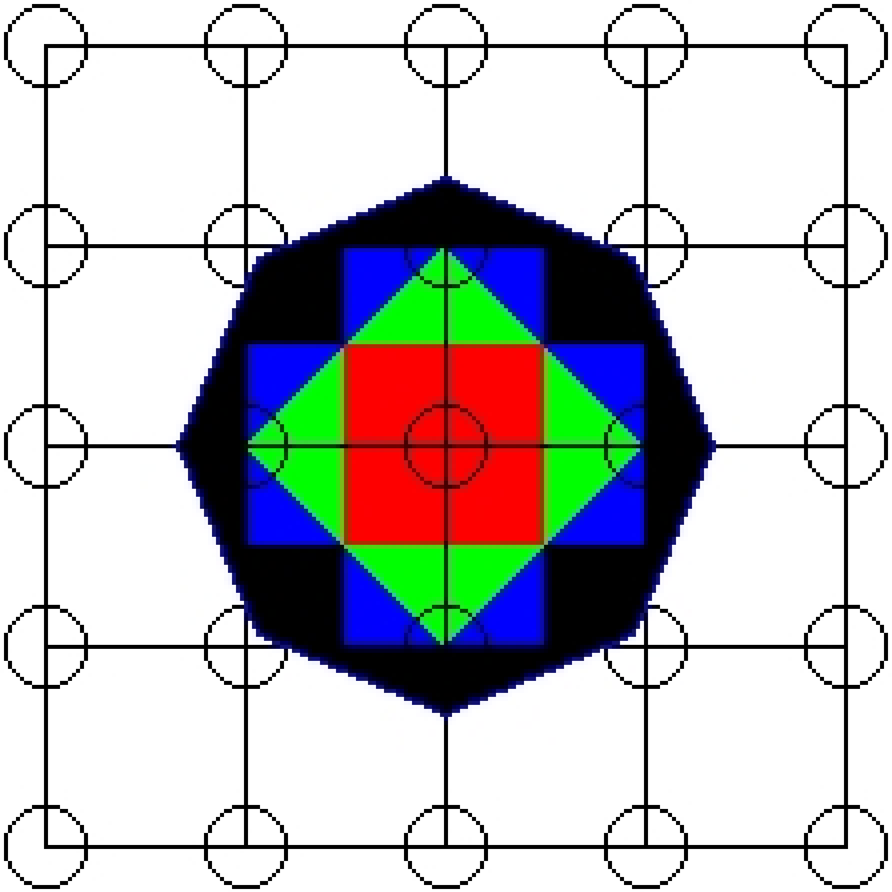
  Bragg reflected

  by the crystal.
- The constructions divide the reciprocal space into fragments, out of which

  The First Brillouin Zone

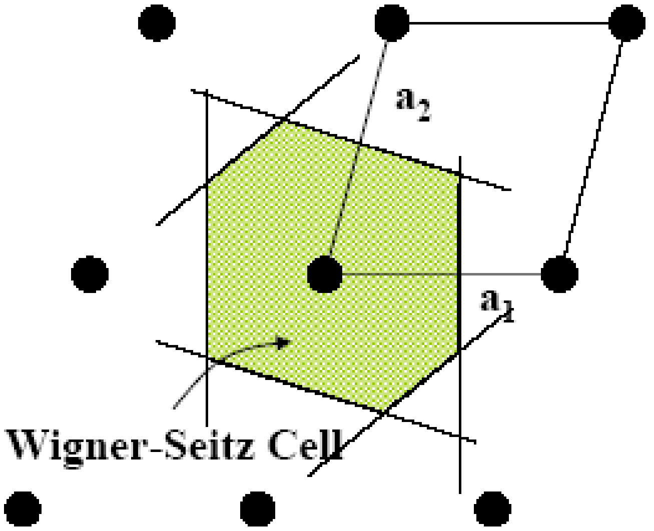
  is of the greatest importance.

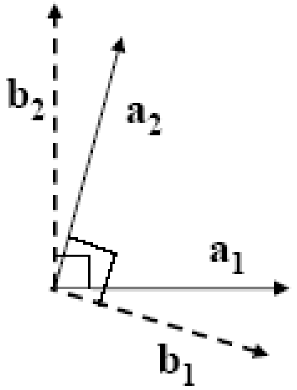
First 4 Brillouin Zones: Square Lattice

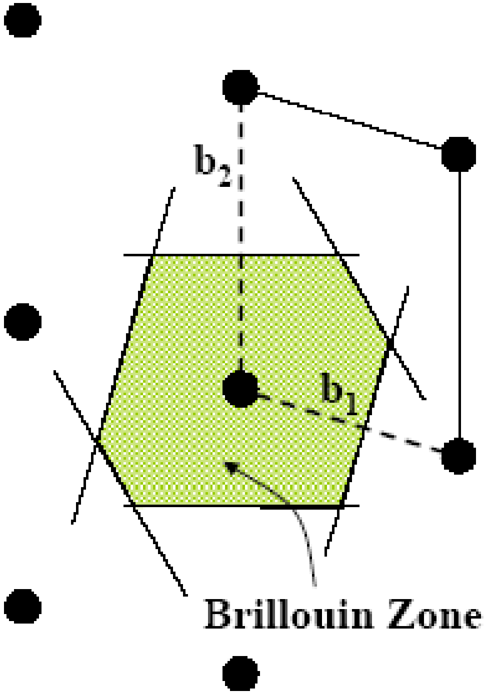


First Four Brillouin Zones for a Square Lattice

Real & Reciprocal lattices in 2 D







$$\mathbf{b}_i = 2\pi \frac{\mathbf{a}_j \times \mathbf{a}_k}{\mathbf{a}_i \cdot \left(\mathbf{a}_j \times \mathbf{a}_k\right)},\ i = x, y, z \rightarrow \mathbf{b}_i \cdot \mathbf{a}_j = 2\pi\delta_{ij}$$

Real & Reciprocal lattices in 2 D

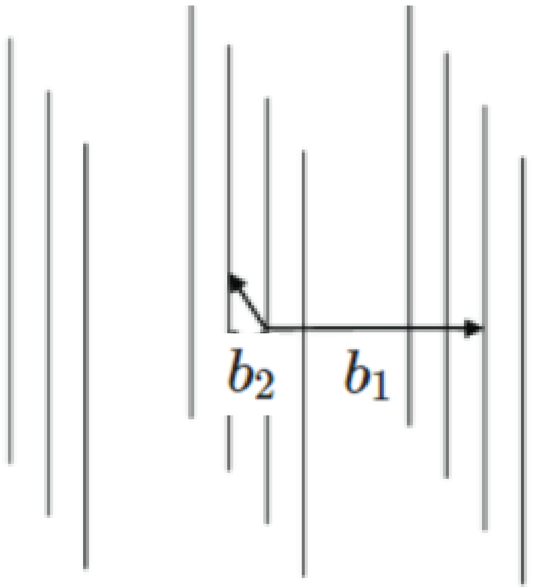
For a 2D square crystal consider $a_1 = a\,\hat{\imath}$, $a_2 = a\,\hat{\jmath}$, and $a_3 = a_3\,\hat{k}$.

Then apply $a_3 \rightarrow 0$, i.e. $b_3 = \infty$

$$b_1 = \frac{2\pi(a_2 \times a_3)}{a_1 . (a_2 \times a_3)}$$

$$b_2 = \frac{2\pi(a_3 \times a_1)}{a_1 . (a_2 \times a_3)}$$

$$b_3 = \frac{2\pi(a_1 \times a_2)}{a_1 . (a_2 \times a_3)}$$

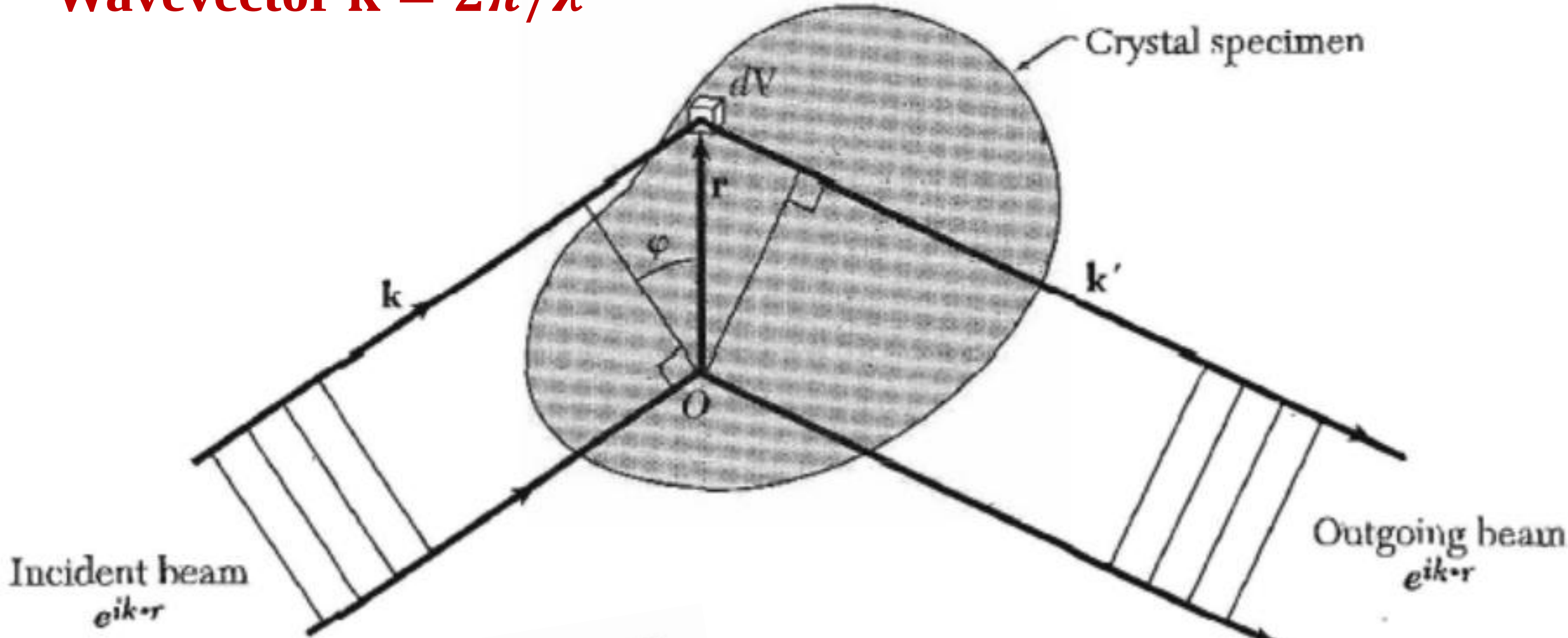


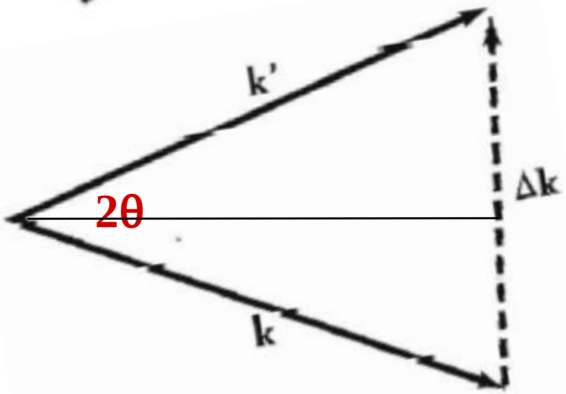
Diffraction Condition (Bragg Law) in the Reciprocal Lattice

- Crystal is composed of identical basis placed at the lattice sites.
- If x-rays are bombarded on the crystal the sharp peaks are observed only in the directions for which the scattered x-rays from the lattice points interfere constructively.
- An **x-ray diffraction** pattern of the lattice ***can be interpreted as a map of the reciprocal lattice of the crystal.***
- This statement is consistent with the following theorem:
- ***The set of Reciprocal Lattice Vectors G determines the possible x-ray reflections.***

Wavevector Representation of X-ray Scattering: $\mathbf{k} \to \mathbf{k}'$

Wavevector $k = 2\pi/\lambda$





$$\boldsymbol{k} + \boldsymbol{\Delta k} = \boldsymbol{k}'$$

For elastic scattering $|\boldsymbol{k}| = |\boldsymbol{k}'|$

$$\Delta \boldsymbol{k} = 2\boldsymbol{k}\,\boldsymbol{sin}\theta$$

Diffraction Condition (Bragg Law) in the Reciprocal Lattice

- X-ray scattered from a volume element is proportional to the local electron concentration $n(r)$.

- The total amplitude (F) of the scattered wave in the direction of k' is proportional to the integral over the crystal of $n(r)dV$ times the phase factor $\exp[i(k-k')\cdot r]$.

$$\boxed{\begin{aligned} F &= \int dV n(\mathbf{r}) e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}} \\ &= \int dV n(\mathbf{r}) e^{-i\Delta\mathbf{k}\cdot\mathbf{r}} \end{aligned}}$$

$$k + \Delta k = k'$$

The ***Δk*** measures the change in wavevector and is called the **scattering vector.**

Using $n(r) \ = \ \Sigma_G n_G e^{\mathrm{i}\,\mathrm{G}\,\cdot\,\mathrm{r}}$, the scattering amplitude becomes.

$$F = \Sigma_G \int dV\, n_G e^{i\,(\mathbf{G} - \Delta\mathbf{k})\cdot\mathbf{r}}$$

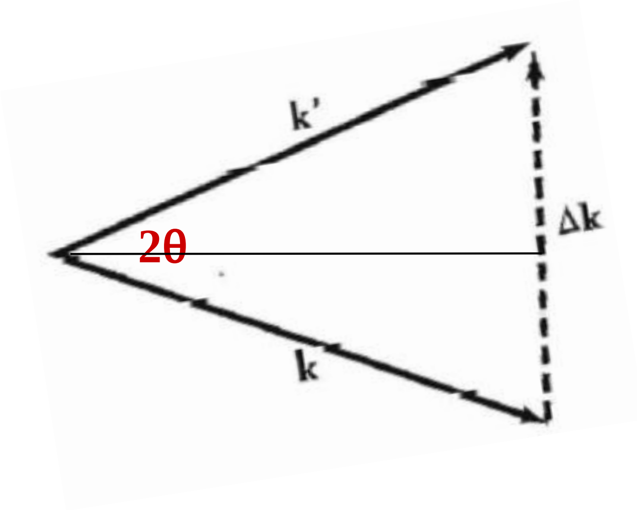
When scattering vector is equal to a particular reciprocal lattice vector:

$$G = \Delta k \ ➔ \ F = V\, n_G$$

F is negligibly small when Δk differs significantly from any reciprocal lattice vector.

Bragg Law

- For elastic scattering $|\boldsymbol{k}| = |\boldsymbol{k}'|$



$$\boldsymbol{k} + \Delta\boldsymbol{k} = \boldsymbol{k}'$$

- When a scattering vector is equal to a particular reciprocal lattice vector,

$$\boldsymbol{G} = \Delta\boldsymbol{k}$$

$$\boldsymbol{k} + \boldsymbol{G} = \boldsymbol{k}'$$

By scalar product, we get

$\mathbf{2}\boldsymbol{k}.\boldsymbol{G} + \boldsymbol{G}^{\mathbf{2}} = \mathbf{0}$, as $|\boldsymbol{k}| = |\boldsymbol{k}'|$

- This result is called ***Bragg Law***.

The Laue Condition

- The result that **Δk** = **G** can also be expressed to give the relations that are called the *Laue Relations* or the *Laue Equations*.
- These are obtained by taking the dot product of

Δk = **G** with $\mathbf{a}_1$, $\mathbf{a}_2$ & $\mathbf{a}_3$.

$$\boxed{\mathbf{G} = v_1\mathbf{b}_1 + v_2\mathbf{b}_2 + v_3\mathbf{b}_3} \qquad \mathbf{b}_i \cdot \mathbf{a}_j = 2\pi\delta_{ij}$$

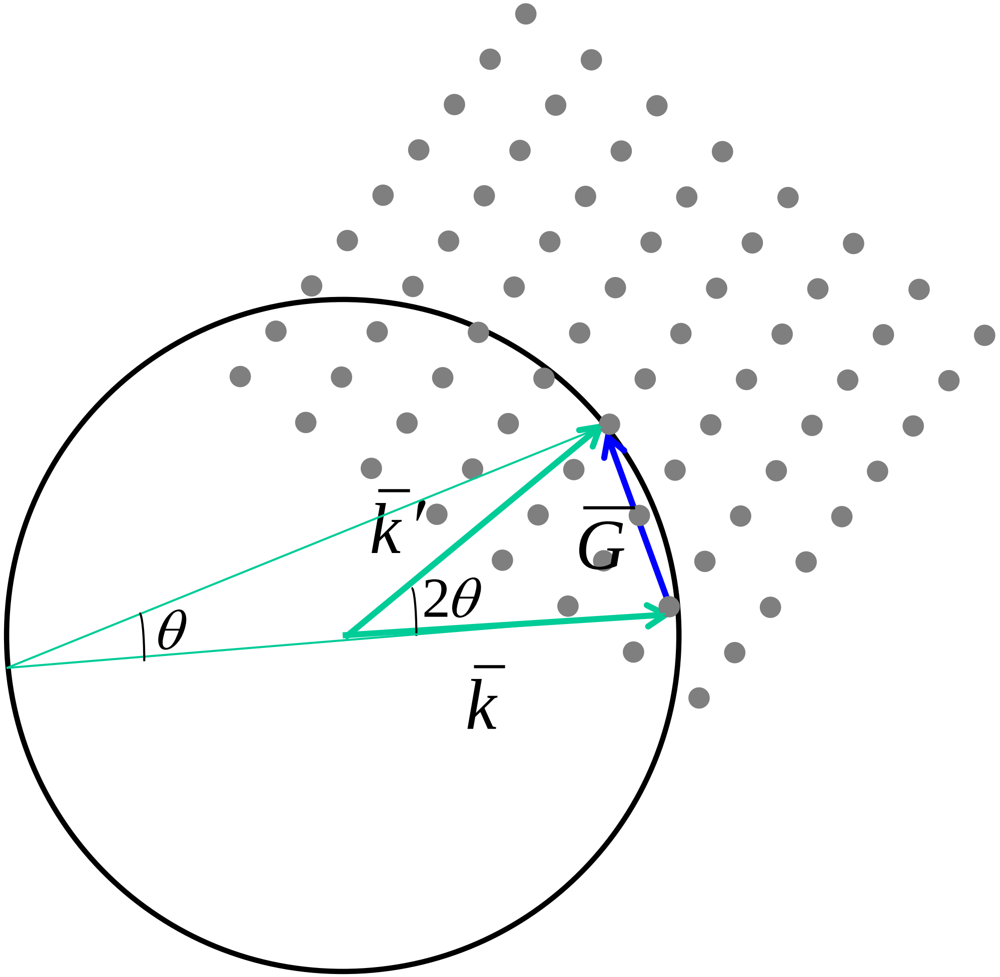
The Laue Equations are:

$$\boxed{\Delta\mathbf{k} \cdot \mathbf{a}_i = 2\pi v_i, \quad i = 1,2,3}$$

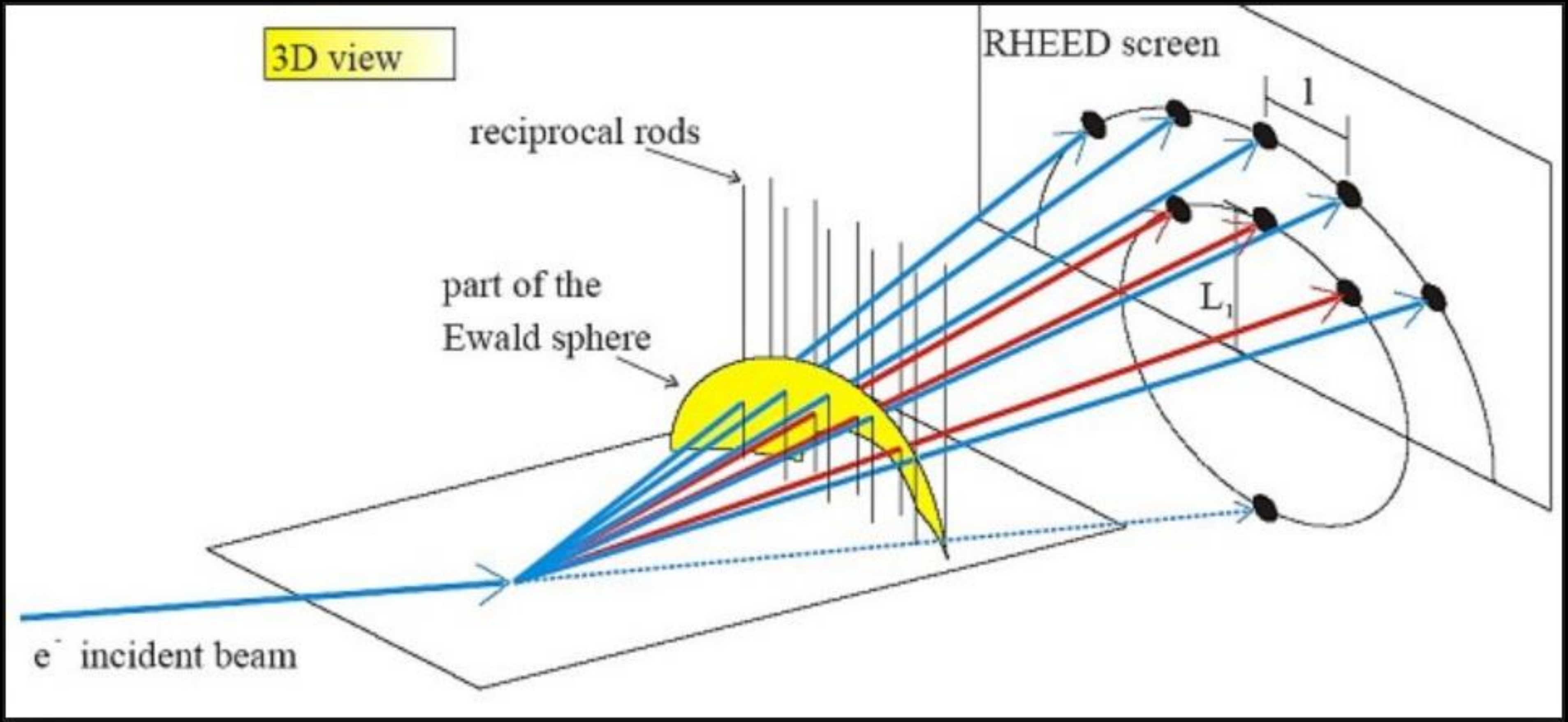
$$\Delta k . a_1 = 2\pi h \qquad \Delta k . a_2 = 2\pi k \qquad \Delta k . a_3 = 2\pi l$$

The Ewald Construction (Circle/Sphere)

- The points in the figure are reciprocal lattice points of the crystal.
- The vector **k** is drawn in the direction of the incident x-ray beam. It terminates at a reciprocal lattice point.
- If we draw a sphere of radius |**k**| about the origin of **k**, then diffracted beam will be formed only if sphere intersects any other reciprocal lattice point.
- The angle θ is the Bragg angle.



Reflection High Energy Electron Diffraction



https://www.wmi.badw.de/methods/leed_rheed.htm

1. **Fourier Analysis of the Basis**

2. **Structure Factor for SC, BCC, and FCC**

- **What property of a basis affects x-ray scattering from the basis?**

- **(size, number of electrons, number of atoms, total mass, density, spin)**

Fourier Analysis of the Basis

Structure Factor & Atomic Form Factor

The scattering amplitude for N unit cells has the form:

$$\mathrm{F}_G = \mathrm{N} \int_{cell} dV\, n(r)\, e^{-i\mathbf{G}\cdot\mathbf{r}} = \mathrm{N}\, \mathrm{S}_G$$

The quantity **S_G** is called ***structure factor***. It is defined as an integral over a single unit cell.

If the electron density is written as a superposition of the electron densities in the cell, taking into account the number of atoms in the basis, it has the form:

$$\boxed{n(\mathbf{r}) = \sum_{j=1}^{s} n_j(\mathbf{r}-\mathbf{r}_j)}$$

where ***s*** is the number of atoms in the basis.

Using this, ***The Structure Factor*** has the form:

$$S_G = \sum_{j=1}^{s} \int_{cell} dV\, n_j(\mathbf{r}-\mathbf{r}_j)\, e^{-i\mathbf{G}\cdot\mathbf{r}}$$

The displacement of one atom in the basis from another atom is $\boldsymbol{r} - \boldsymbol{r_j} = \boldsymbol{\rho}$, so that $\boldsymbol{r} = \boldsymbol{\rho} + \boldsymbol{r_j}$

$$= \sum_{j=1}^{s} e^{-i\mathbf{G}\cdot\mathbf{r}_j} \int_{cell} dV\, n_j(\rho)\, e^{-i\mathbf{G}\cdot\rho} = \sum_{j=1}^{s} e^{-i\mathbf{G}\cdot\mathbf{r}_j} f_j$$

The quantity f_j is called ***The Atomic Form Factor***.

From the earlier equation the atomic form factor is:

$$f_j = \int dV n_j(\bar{\rho}) \exp(-i\bar{G}.\bar{\rho})$$

- If (& only if!) ***the electron density of the atom is spherically-symmetric***,
- Volume element in spherical coordinates is:

$$dV = d\rho\, \rho^2 d(cos\alpha) d\phi$$

$$f_j = \int_0^{2\pi} d\phi \int_0^{\rho} d\rho \int_{-1}^{1} \rho^2 d(cos\alpha) n_j(\rho) exp(-iG\rho cos\alpha)$$

$$f_j = 2\pi \int_0^{\rho} d\rho\, \rho^2 n_j(\rho)\, \frac{exp(iG\rho) - exp(-iG\rho)}{iG\rho}$$

$$f_j = 4\pi \int_0^{\rho} d\rho\, \rho^2 n_j(\rho)\, \frac{\sin(G\rho)}{G\rho}$$

If electron were concentrated at $\rho = 0$, only $G\rho = 0$ would contribute to the integrand, and $n_j(\rho)$ will have a constant value.

$$\lim_{G\rho \to 0} sin(G\rho)/G\rho = 1$$

$$f_j = 4\pi n_j \int_0^{\rho} d\rho\, \rho^2 = \frac{4\pi}{3}\rho^3 n_j = Z$$

- where Z is atomic number of a single atom in the basis or the sum of all electrons of many atoms in the basis.

- That is, in this case, f_j is ***the ratio of radiation amplitude scattered by the electron distribution to that scattered by one electron localized at a point.***

To determine the structure factor, we are specifying **G** and $\mathbf{r}_j$ as

$$\mathbf{G} = v_1\mathbf{b}_1 + v_2\mathbf{b}_2 + v_3\mathbf{b}_3 \quad \text{and} \quad \mathbf{r}_j = x_j\mathbf{a}_1 + y_j\mathbf{a}_2 + z_j\mathbf{a}_3$$

where x_j, y_j, and z_j are coordinates of j basis and v_1, v_2, and v_3 are Miller indices.

gives:

$$S_G = \sum_{j=1}^{s} f_j e^{-2\pi i\left(x_j v_1 + y_j v_2 + z_j v_3\right)}$$

Note that S_G can be complex, but the scattering intensity is real because it involves the magnitude squared of $S_G^*.S_G$.

Structure Factor Calculations for Simple cubic lattice

$$\boxed{S_G = \sum_{j=1}^{s} f_j e^{-2\pi i\left(x_j v_1 + y_j v_2 + z_j v_3\right)}}$$

In a **SC lattice**, basis are located at **(000) i.e. x = 0, y = 0, and z = 0**. The structure factor is then:

$$S_G = f$$

This structure factor is equal to atomic form factor *f* for any set (even or odd) of Miller indices.

$$\upsilon_1 + \upsilon_2 + \upsilon_3 = 2n \ (n = \text{integer})$$

$$\upsilon_1 + \upsilon_2 + \upsilon_3 = 2n + 1 \ (n = \text{integer})$$

In XRD pattern, all planes (100), (110), (111) etc will produce peaks.

Structure Factor Calculations for BCC lattice

$$\boxed{S_G = \sum_{j=1}^{s} f_j e^{-2\pi i\left(x_j v_1 + y_j v_2 + z_j v_3\right)}}$$

In a BCC lattice, there are 2 atoms per cubic unit cell located at (000) & (½½ ½). The structure factor is then:

$$\boxed{S_G = \left[1 + e^{-\pi i\left(v_1 + v_2 + v_3\right)}\right] f}$$

$$S_G = \left[1 + \cos\left(\pi(v_1 + v_2 + v_3)\right) + i\sin\left(\pi(v_1 + v_2 + v_3)\right)\right] f$$

$S_G = 2f$ for $\upsilon_1 + \upsilon_2 + \upsilon_3 = 2n$ (n = integer)

$S_G = 0$ for $\upsilon_1 + \upsilon_2 + \upsilon_3 = 2n + 1$ (n = integer)

In XRD pattern, the (110) and (420) planes will produce peaks and there will be no peaks associated with (100), (111) etc planes.

(100) Reflection vanishes in BCC lattice

The (100) reflection occurs in the simple cubic lattice when reflection from the planes that bound the cubic cell differ in phase by 2π.

In the BCC lattice, there is an intervening plane of atoms, which is equal in scattering power as the other planes.

This plane gives a reflection retarded in phase by π with respect to the neighboring plane, so resulting in destructive interference.

Structure Factor Calculations for FCC lattice

For a FCC lattice, there are 4 atoms per cubic unit cell located at (000), (0½½), (½ 0½) & (½½0). The structure factor is then:

$$\boxed{S_G = \left[1 + e^{-\pi i(v_1+v_2)} + e^{-\pi i(v_1+v_3)} + e^{-\pi i(v_2+v_3)}\right] f}$$

This structure factor has its *Maximum value* $S_G = 4f$ when *all indices* υ_1, υ_2, υ_3 *are even or odd* such as (111) or (420).

This structure factor *Vanishes*, $S_G = 0$ when *the indices are partially even & partially odd* such as (120) or (421).

In XRD pattern, the (111) and (420) planes will produce peaks and there will be no peaks associated with (120), (421) etc planes.

Observed & Calculated

Atomic Form Factor for Aluminium

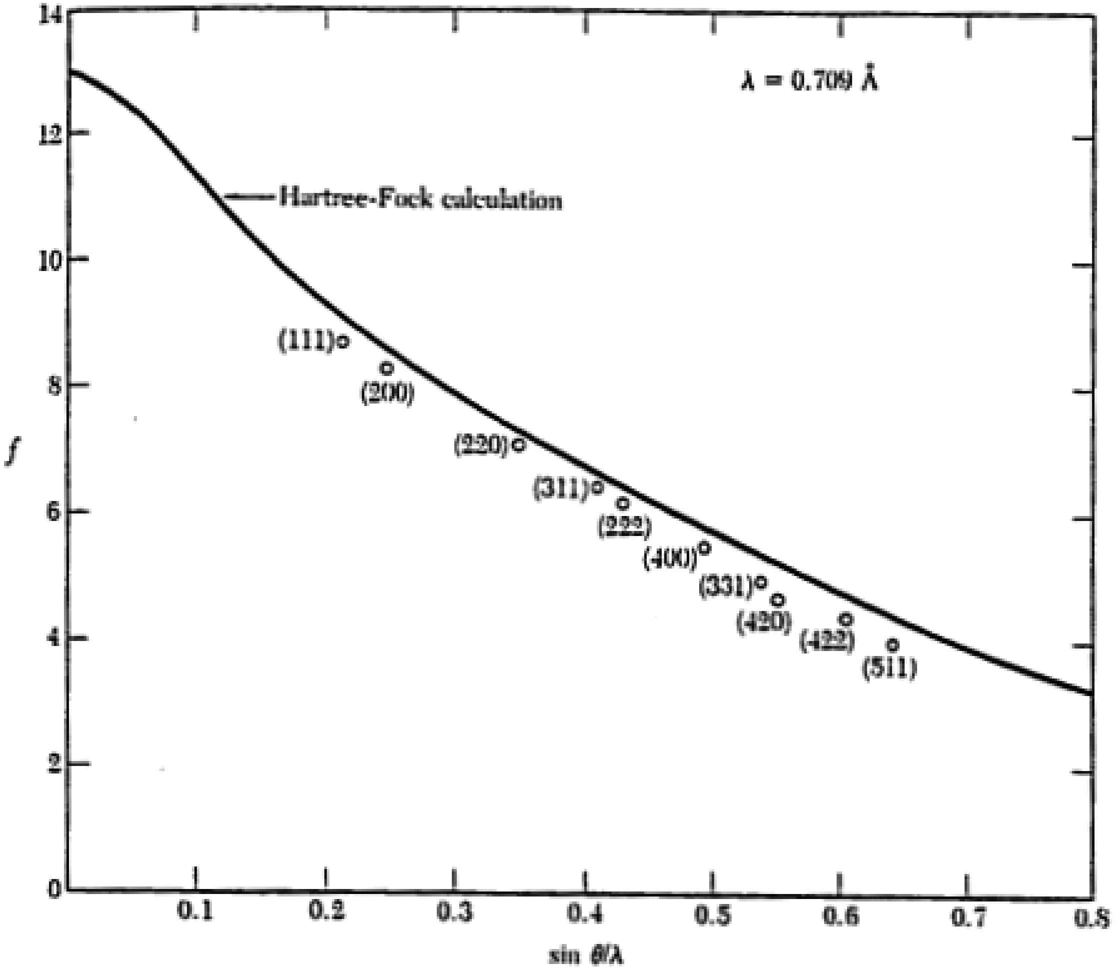
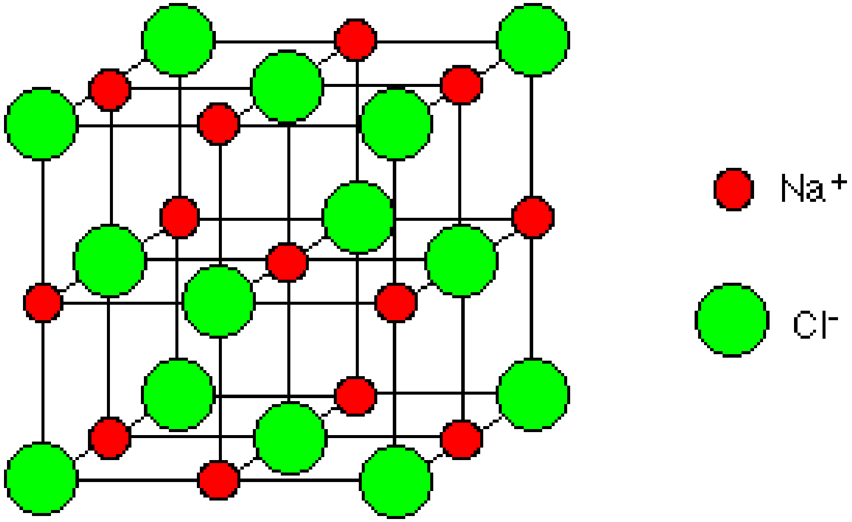
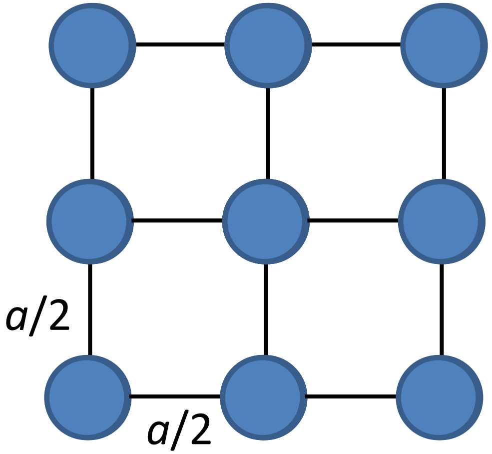


Figure 18 Absolute experimental atomic scattering factors for metallic aluminum, after Batterman, Chipman, and DeMarco. Each observed reflection is labeled. No reflections occur for indices partly even and partly odd, as predicted for an fcc crystal.

Difference in XRD spectra of KCl and KBr

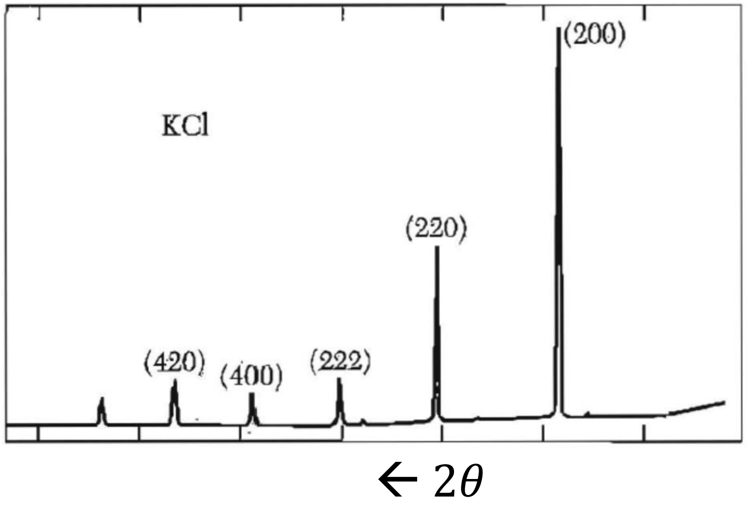
Both KCl and KBr have rock salt crystal structure, but n(**r**) for KCl simulates as SC lattice because the atomic number of K and Cl atoms are 19 and 17, respectively and ions have equal number of electrons (18). Whereas the electrons in Br (z=35) are significantly larger than in K.



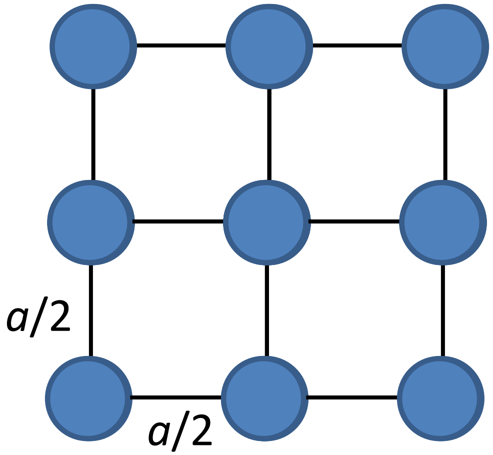


Difference in XRD spectra of KCl and KBr

The scattering amplitudes f(K+) and f(Cl-) are almost exactly equal.



so crystal looks to x-rays as if it were a monatomic simple cubic lattice of lattice constant *a*/2.



Only even integers occur in the reflection indices when they are based on a cubic lattice of lattice constant *a/2*.

Difference in XRD spectra of KCl and KBr

In KBr the form factor of Br^- is quite different to that of K^+, and all reflections of the FCC lattice are present