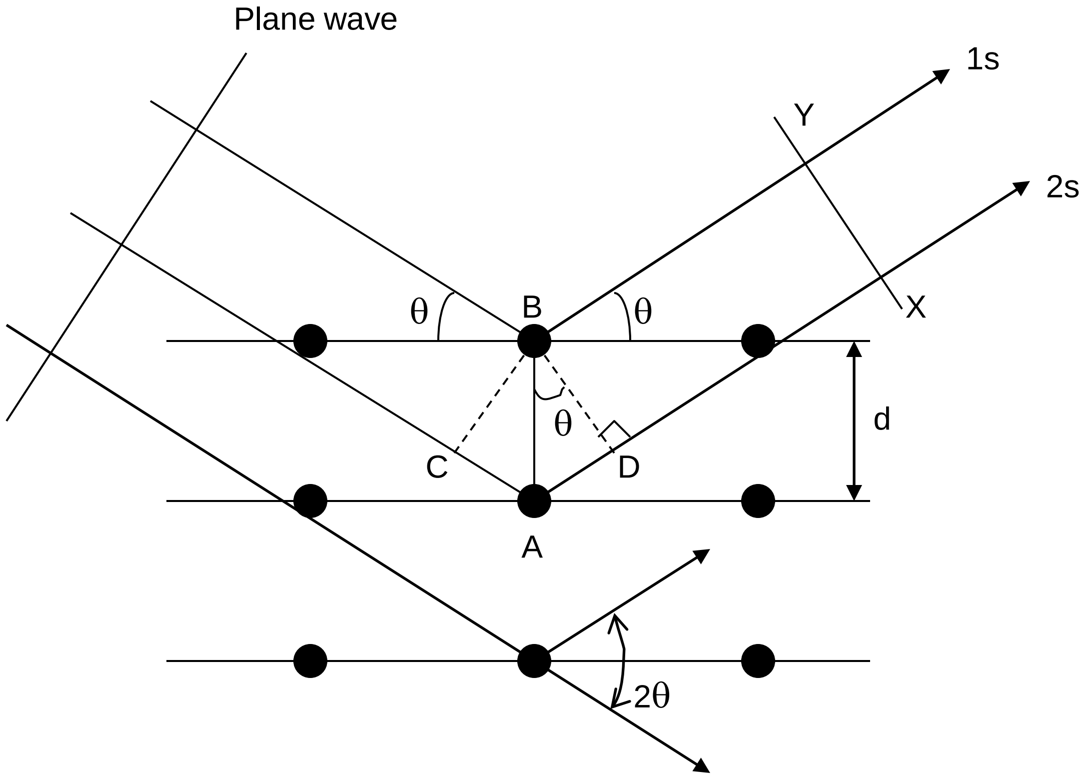
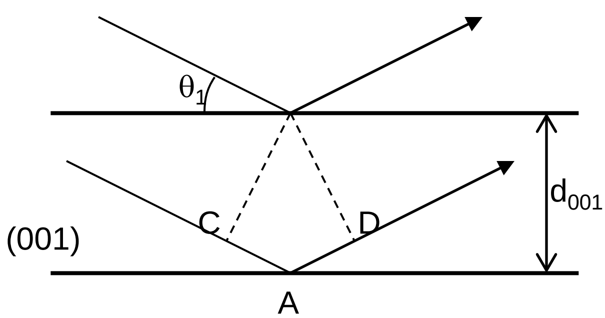
1. Bragg Condition

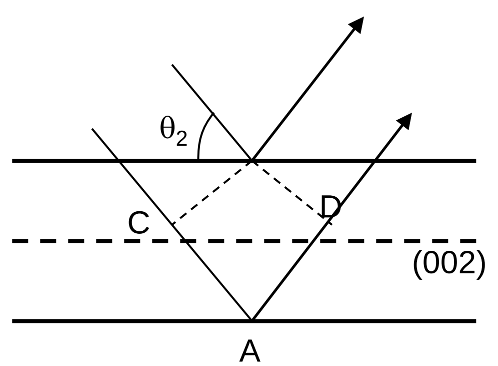


The path difference between 1s and 2s = CA + AD = d sinθ + d sinθ = 2d sinθ

If this path difference is a multiple of λ, the scattered waves 1s and 2s are in phase, resulting in a diffraction.

$$2d \sin\theta = n\lambda, \quad \text{where } n \text{ is an integer}$$





CA + AD = λ $\quad$ $2d_{001} \sin\theta_1 = \lambda$

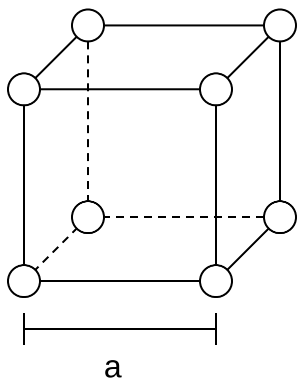
CA + AD = 2λ $\quad$ $2d_{001} \sin\theta_2 = 2\lambda$

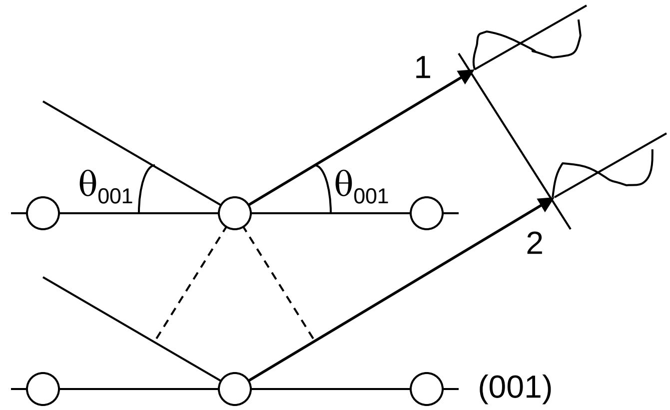
$$2\,\frac{d_{001}}{2} \sin\theta_2 = \lambda = 2d_{002} \sin\theta_2$$

Bragg condition: $\lambda = 2d \sin\theta$

- Three cubic crystals with an identical lattice constant a.
  For (001) diffraction, $\lambda = 2a \sin \theta_{001}$

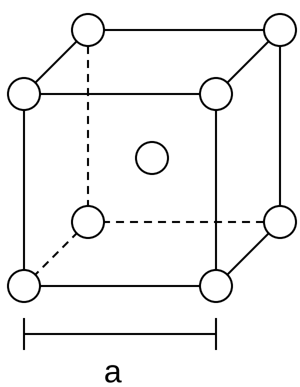
i) Simple cubic

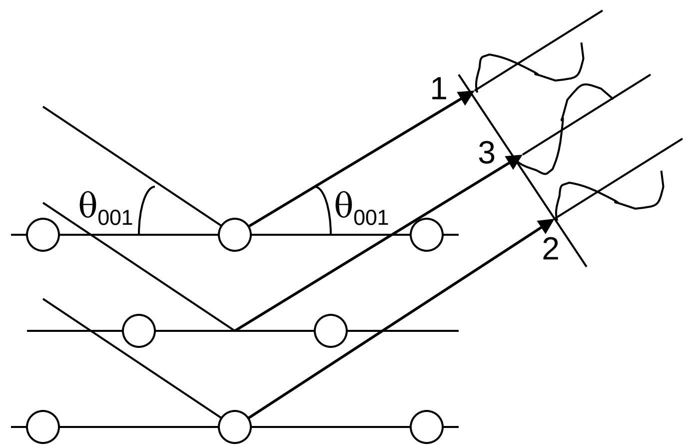




1 and 2 are in phase

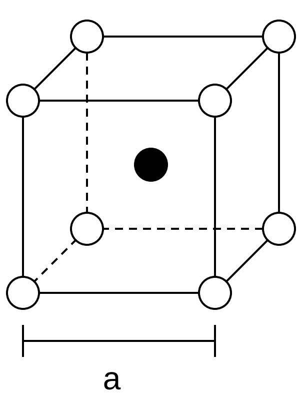
ii) Body-centered cubic

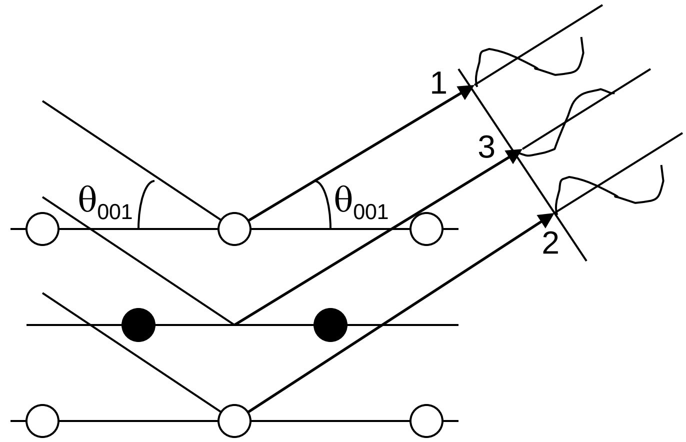




1 and 3 are out of phase, I_{001} goes to zero

ii) Simple cubic(CsCl)

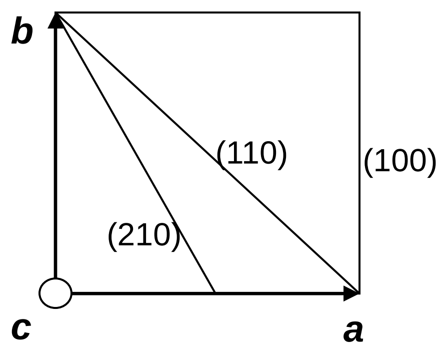




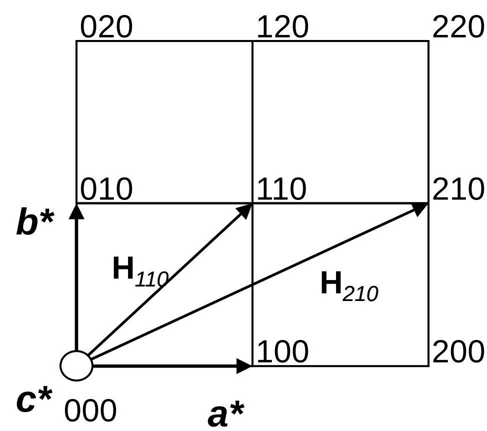
1 and 3 are out of phase, but I_{001} may not go to zero

2. Vectors in Reciprocal Lattice, $\mathbf{H}_{hkl}$

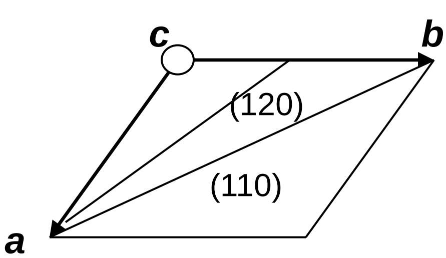
$$\mathbf{H}_{hkl} = h\boldsymbol{a}^* + k\boldsymbol{b}^* + l\boldsymbol{c}^*$$

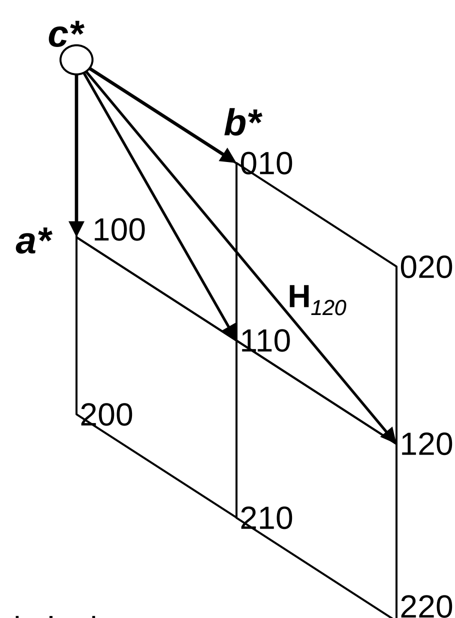


Lattice



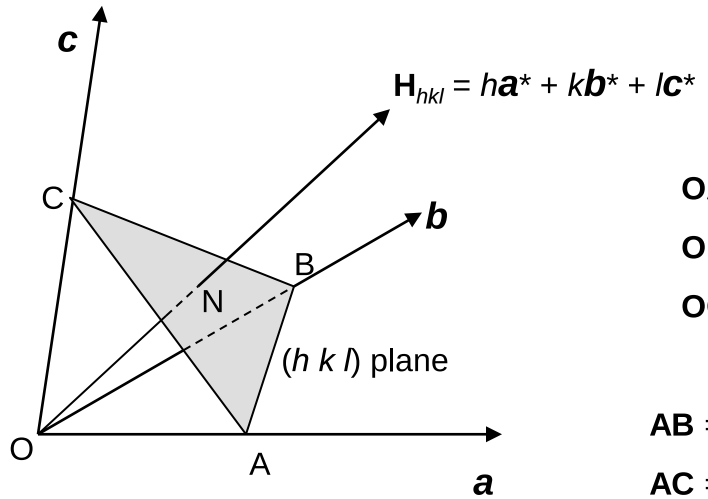
Reciprocal Lattice





- $\mathbf{H}_{hkl}$ is perpendicular to the (h k l) plane in lattice

- $H_{hkl} = |\mathbf{H}_{hkl}| = \dfrac{1}{d_{hkl}}$



OA = $\boldsymbol{a}/h$

OB = $\boldsymbol{b}/k$

OC = $\boldsymbol{c}/l$

AB = **OB – OA** = $\boldsymbol{b}/k - \boldsymbol{a}/h$

AC = **OC – OA** = $\boldsymbol{c}/l - \boldsymbol{a}/h$

$$\mathbf{H} \cdot \mathbf{AB} = (h\boldsymbol{a}^* + k\boldsymbol{b}^* + l\boldsymbol{c}^*) \cdot (\boldsymbol{b}/k - \boldsymbol{a}/h) = -\,\boldsymbol{a}^* \cdot \boldsymbol{a} + \boldsymbol{b}^* \cdot \boldsymbol{b} = -1 + 1 = 0$$

$$\mathbf{H} \cdot \mathbf{AC} = (h\boldsymbol{a}^* + k\boldsymbol{b}^* + l\boldsymbol{c}^*) \cdot (\boldsymbol{c}/l - \boldsymbol{a}/h) = -\,\boldsymbol{a}^* \cdot \boldsymbol{a} + \boldsymbol{c}^* \cdot \boldsymbol{c} = -1 + 1 = 0$$

H is normal to both **AB** and **AC**, so it is also normal to (h k l) plane.

$$d_{hkl} = \mathrm{ON} = \mathbf{OA} \cdot \frac{\mathbf{H}_{hkl}}{H_{hkl}} = \boldsymbol{a}/h \cdot \frac{(h\boldsymbol{a}^* + k\boldsymbol{b}^* + l\boldsymbol{c}^*)}{H_{hkl}} = \frac{1}{H_{hkl}}$$

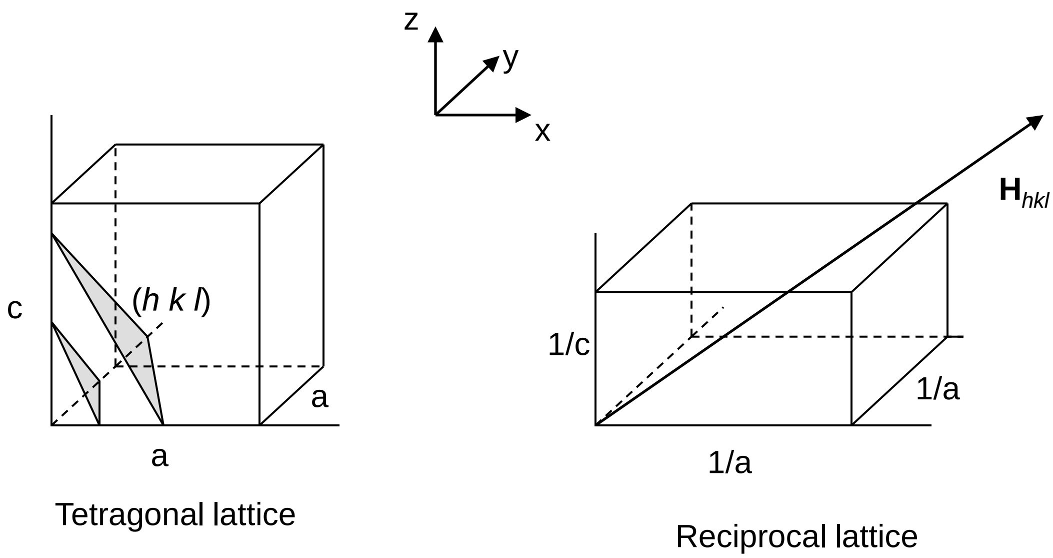
In Cubic Crystals (a = b = c, $\alpha = \beta = \gamma = 90^{o}$)

$$|\boldsymbol{a}^*| = |\boldsymbol{b}^*| = |\boldsymbol{c}^*| = 1/a$$

$$H_{hkl} = \frac{(h^2 + k^2 + l^2)^{1/2}}{a} \qquad d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

In Tetragonal Crystals (a = b ‡ c, $\alpha = \beta = \gamma = 90^o$)

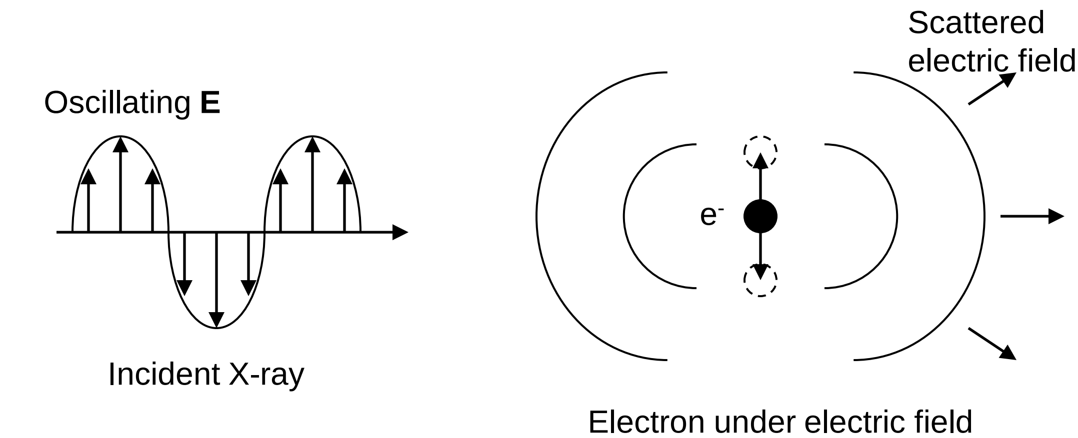
$|\boldsymbol{a^*}| = |\boldsymbol{b^*}| = 1/a$, $|\boldsymbol{c^*}| = 1/c$



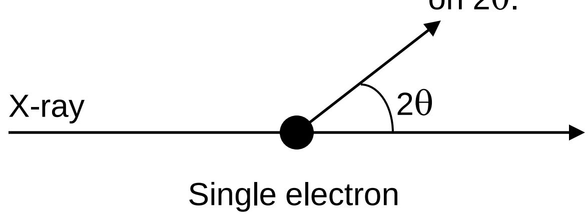
$$H_{hkl} = \sqrt{(h/a)^2 + (k/a)^2 + (l/c)^2}$$

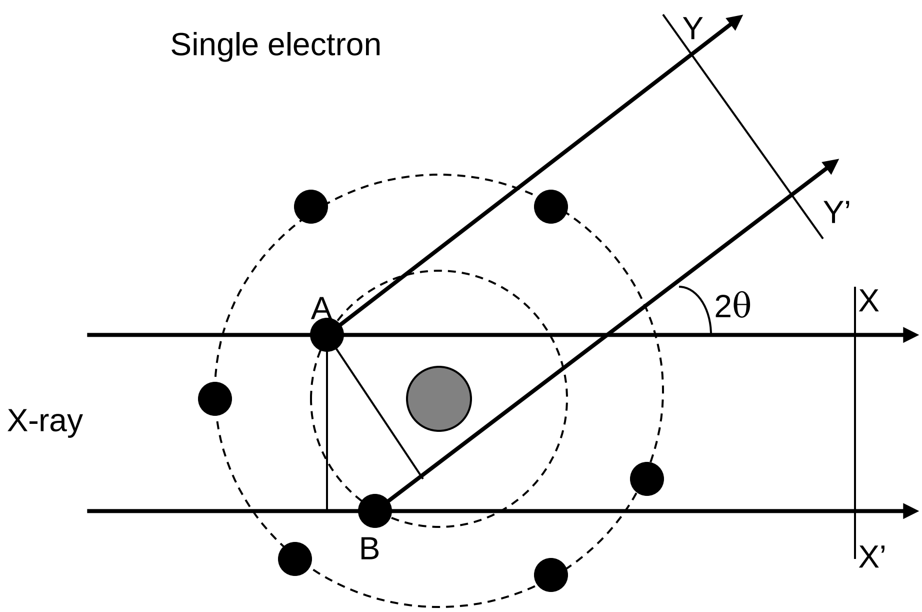
$$d_{hkl} = 1/\,H_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2\,(a/c)^2}}$$

3. Scattering by an Electron and an Atom



The amplitude of scattered wave, E_e, depends on 2θ.





The total electric field of scattered waves on Y-Y' is the sum of the waves scattered by individual electrons.

$$E_{Y\text{-}Y'} = E_e\cos(2\pi x/\lambda - \delta_1) + E_e\cos(2\pi x/\lambda - \delta_2) + \ldots E_e\cos(2\pi x/\lambda - \delta_z)$$

Z: Atomic number

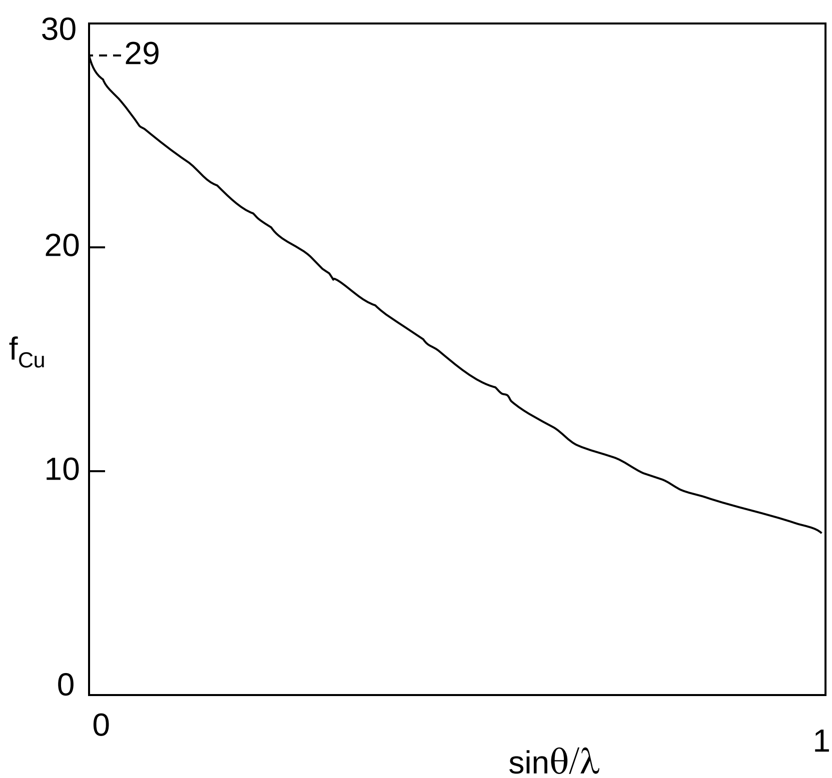
$$E_{Y\text{-}Y'} = E_e \cos(2\pi x/\lambda - \delta_1) + E_e \cos(2\pi x/\lambda - \delta_2) + \ldots E_e \cos(2\pi x/\lambda - \delta_z)$$
$$= E_{atom} \cos(2\pi x/\lambda - \delta_t)$$

E_{atom}: The amplitude of scattered wave by an atom ($0 < E_{atom} \leq ZE_e$)

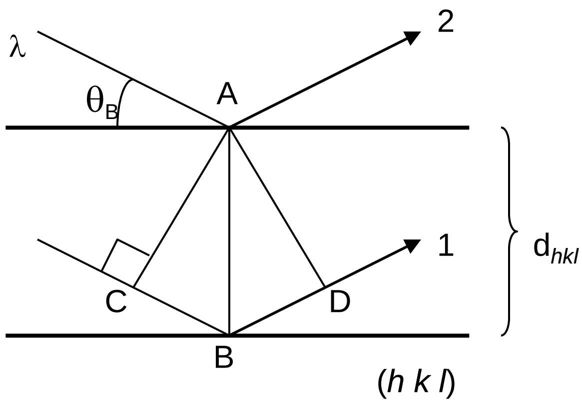
If 2θ is zero, $\delta_1 = \delta_2 = \ldots.. = \delta_z$, then $E_{atom} = ZE_e$

Atomic scattering factor, *f*

$$f = \frac{\text{Amplitude of the wave scattered by an atom}}{\text{Amplitude of the wave scattered by an electron}} = \frac{E_{atom}}{E_e}$$



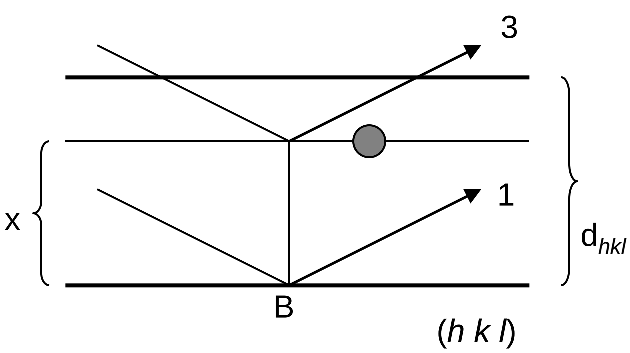
4. Scattering by a Unit Cell



For Bragg-Matched, $\lambda = 2d_{hkl}\sin\theta_B$

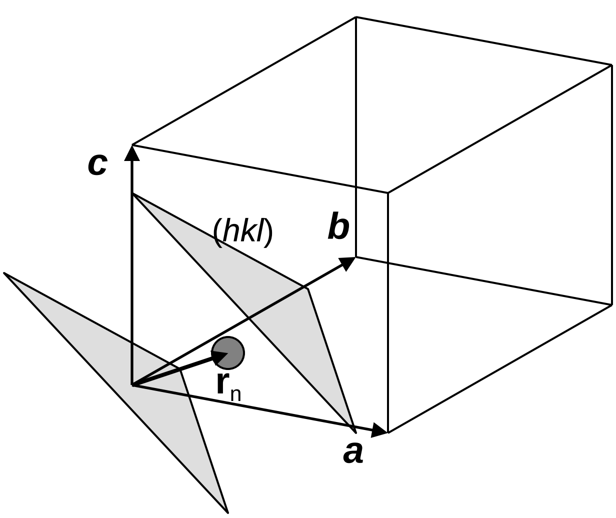
Path difference between 1 and 2 is CB + BD = λ =2d$\sin\theta_B$

$$\text{Phase difference } \delta = \frac{2\pi}{\lambda}(CB + BD)$$
$$= 2\pi$$

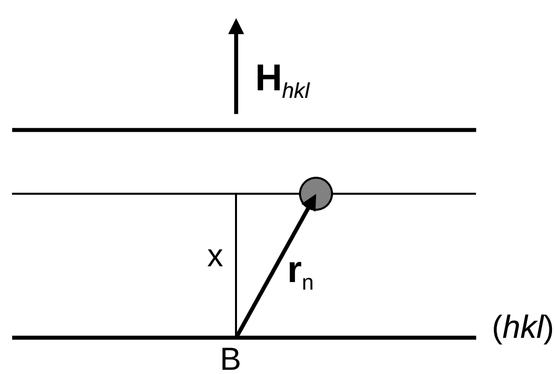


Path difference between 1 and 3 is $\frac{x}{d_{hkl}}\lambda$

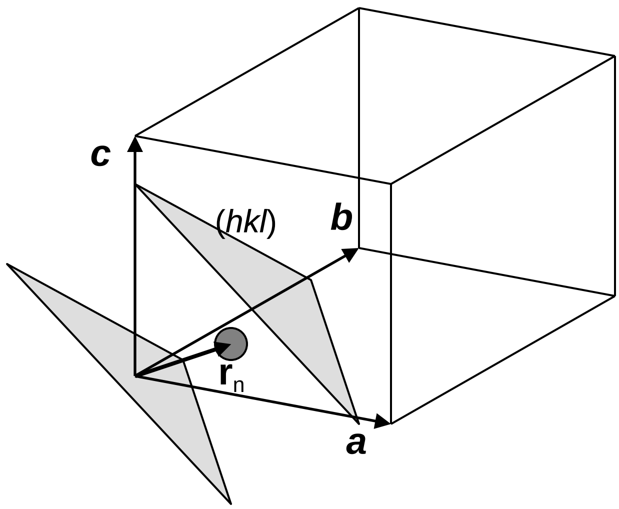
$$\text{Phase difference } \delta = \frac{2\pi}{\lambda}\frac{x}{d_{hkl}}\lambda$$
$$= \frac{2\pi x}{d_{hkl}}$$



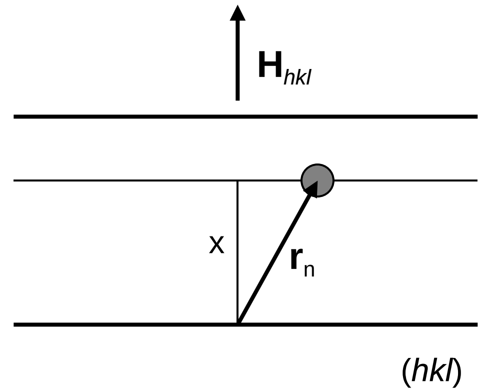
$\mathbf{r}_n = u\boldsymbol{a} + v\boldsymbol{b} + w\boldsymbol{c}$



$$x = \frac{\mathbf{H}_{hkl}}{H_{hkl}} \cdot \mathbf{r}_n$$



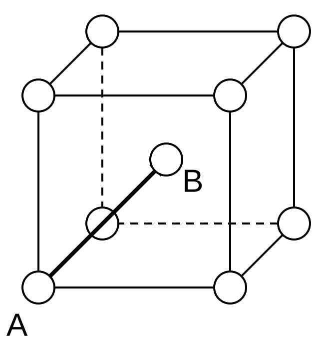
$$\mathbf{r}_n = u\boldsymbol{a} + v\boldsymbol{b} + w\boldsymbol{c}$$

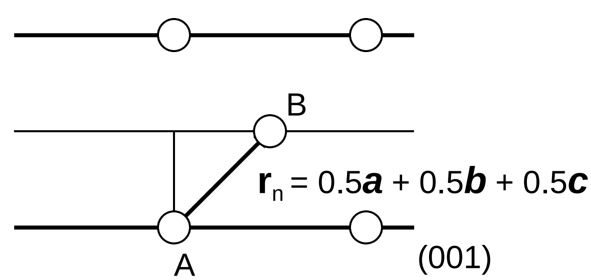


$$x = \frac{\mathbf{H}_{hkl}}{H_{hkl}} \cdot \mathbf{r}_n$$

$$\text{Phase difference } \delta = \frac{2\pi x}{d_{hkl}} = \frac{2\pi}{d_{hkl}} \frac{\mathbf{H}_{hkl}}{H_{hkl}} \cdot \mathbf{r}_n = 2\pi\, \mathbf{H}_{\mathrm{hkl}} \cdot \mathbf{r}_n$$
$$= 2\pi(hu + kv + lw)$$

e.g., Body-centered cubic, (001) diffraction.

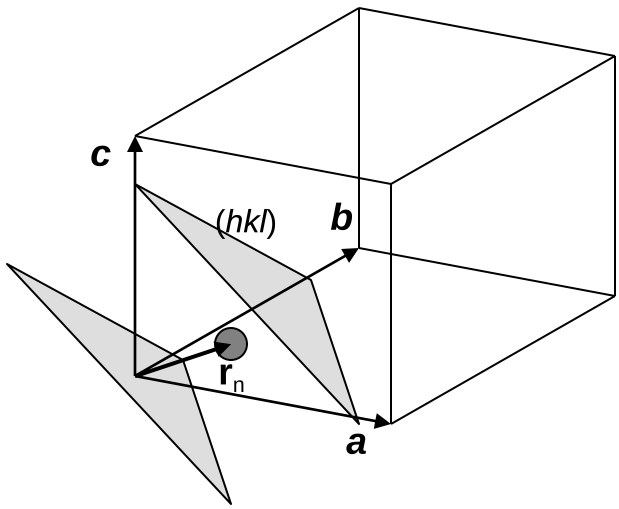




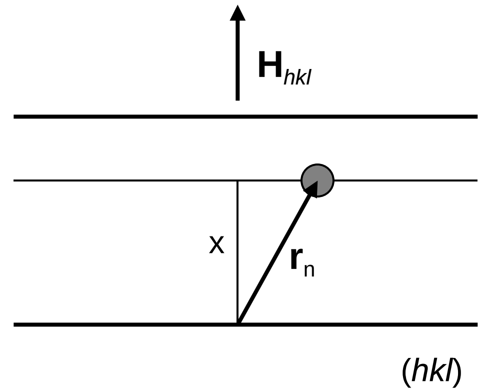
$$\delta = 2\pi\,(\boldsymbol{c}^*) \cdot (0.5\boldsymbol{a} + 0.5\boldsymbol{b} + 0.5\boldsymbol{c}) = \pi\, \boldsymbol{c}^* \cdot \boldsymbol{c} = \pi$$

If the wave scattered from atom A is $f_A\cos(2\pi x/\lambda)$, then the wave scattered from atom B is $f_B\cos(2\pi x/\lambda - \pi)$, where $f_A = f_B$

⇨ The (001) diffraction intensity will be zero.



$\mathbf{r}_n = u\boldsymbol{a} + v\boldsymbol{b} + w\boldsymbol{c}$



$$x = \frac{\mathbf{H}_{hkl}}{H_{hkl}} \cdot \mathbf{r}_n$$

$$\text{Phase difference } \delta = \frac{2\pi x}{d_{hkl}} = \frac{2\pi}{d_{hkl}} \frac{\mathbf{H}_{hkl}}{H_{hkl}} \cdot \mathbf{r}_n = 2\pi\, \mathbf{H}_{\mathrm{hkl}} \cdot \mathbf{r}_n$$

$$= 2\pi(hu + kv + lw)$$

- Scattering by a unit cell for (h k l) diffraction

If a unit cell contains atoms, 1, 2, 3, N, with fractional coordinates (u_1, v_1, w_1), (u_2, v_2, w_2), …. (u_N, v_N, w_N), the total scattered wave can be represented by

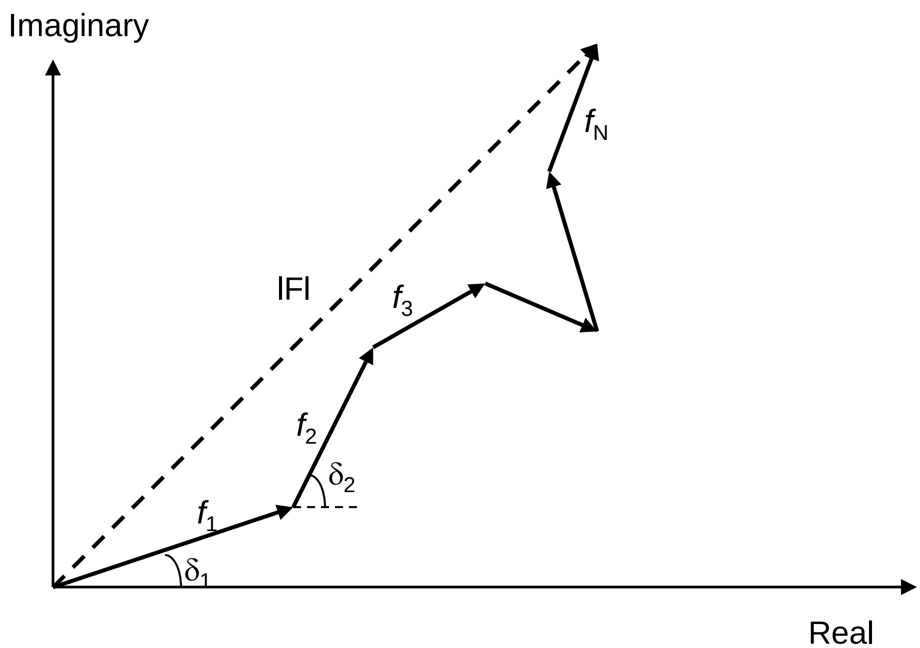
$$F = f_1 e^{i\delta 1} + f_2 e^{i\delta 2} + \ldots.\ f_N e^{i\delta N}$$

$$= f_1 \exp\{2\pi i(hu_1 + kv_1 + lw_1)\} + \ldots + f_N \exp\{2\pi i(hu_N + kv_N + lw_N)\}$$

$$F_{hkl} = \sum_{1}^{N} f_n \exp\{2\pi i(hu_n + kv_n + lw_n)\} \quad \Leftarrow \quad \text{Structure factor}$$

$F = f_1 e^{i\delta 1} + f_2 e^{i\delta 2} + \ldots. f_N e^{i\delta N}$

$= f_1 \exp\{2\pi i(hu_1 + kv_1 + lw_1)\} + \ldots + f_N \exp\{2\pi i(hu_N + kv_N + lw_N)\}$

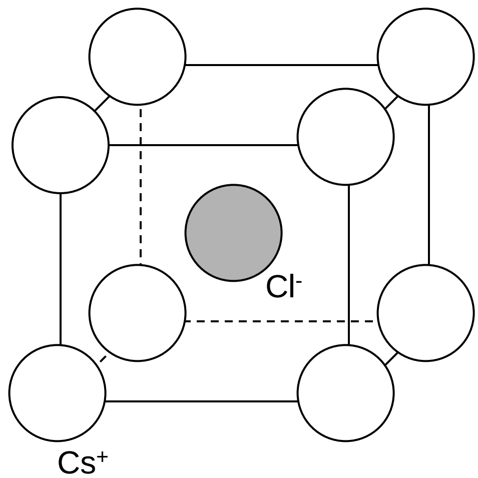


$$|F_{hkl}| = \frac{\text{Amplitude of the wave scattered by a unit cell}}{\text{Amplitude of the wave scattered by an electron}}$$

The intensity of the beam diffracted by all the atoms of the unit cell in a direction satisfying the Bragg condition is proportional to $|F_{hkl}|^2$, that is.,

$$I \propto |F_{hkl}|^2$$

Example 1: CsCl Structure

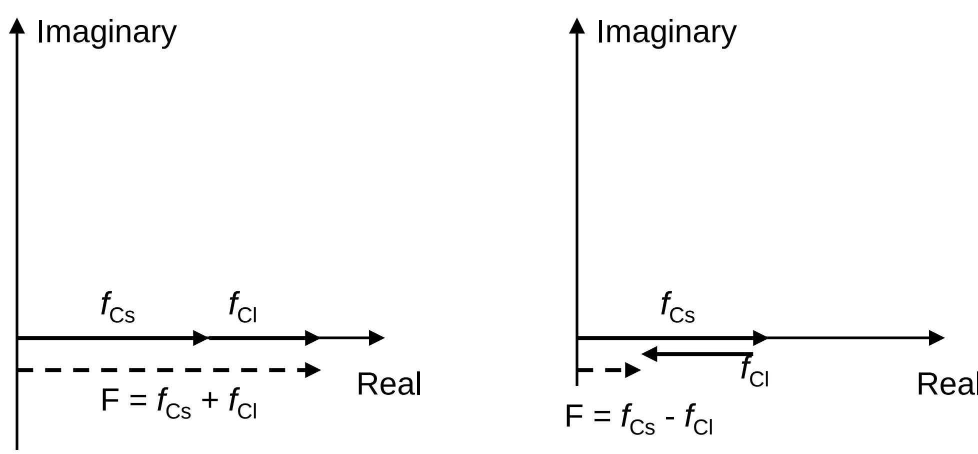


Coordinate: Cs^+ (0, 0, 0), Cl^- (½, ½, ½)

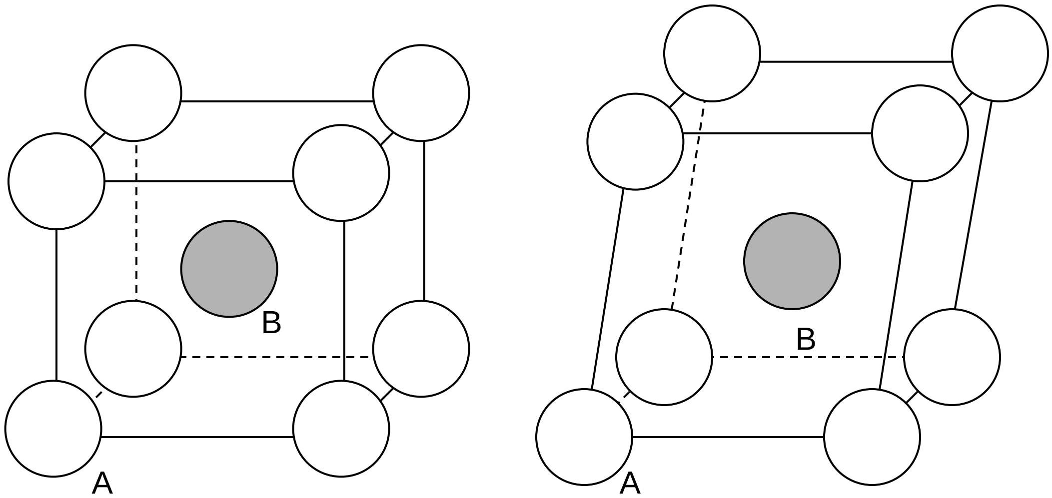
$$F = f_{Cs} + f_{Cl}\, e^{\pi i(h + k + l)}$$

If $h + k + l$ are even, $F = f_{Cs} + f_{Cl}$, $F^2 = (f_{Cs} + f_{Cl})^2$

If $h + k + l$ are odd, $F = f_{Cs} - f_{Cl}$, $F^2 = (f_{Cs} - f_{Cl})^2$



Example 2: AB compound with the different shape and size of the unit cell



Coordinates: A (0, 0, 0), B (½, ½, ½)

$$F = f_A + f_B e^{\pi i(h + k + l)}$$

If $h + k + l$ are even, $F = f_A + f_B$, $F^2 = (f_A + f_B)^2$

If $h + k + l$ are odd, $F = f_A - f_B$, $F^2 = (f_A - f_B)^2$

* Structure factor F is independent of the shape and size of the unit cell.

Important Remarks:

1. The diffraction direction is determined by the Bragg condition, which is affected by the shape and size of the unit cell.

2. The diffraction intensity is independent of the shape and size of the unit cell, only affected by the atomic arrangement within the unit cell.