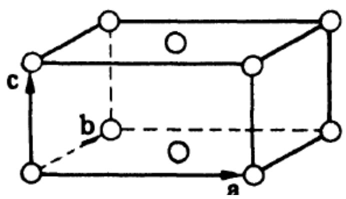
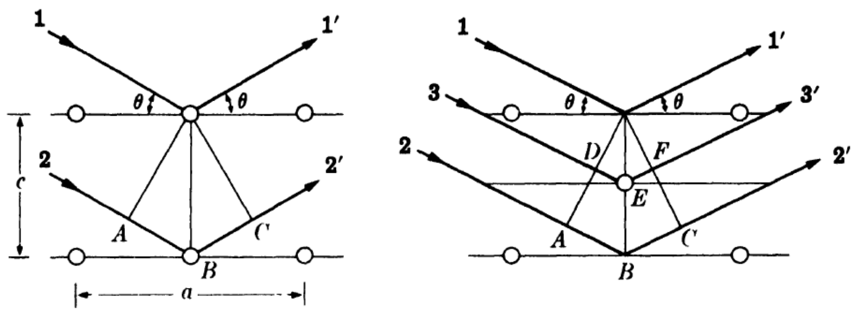
Röntgenbeugung-Intensität (II):

- The positions of the atoms in the unit cell affect the intensities but not the directions of the diffracted beams.



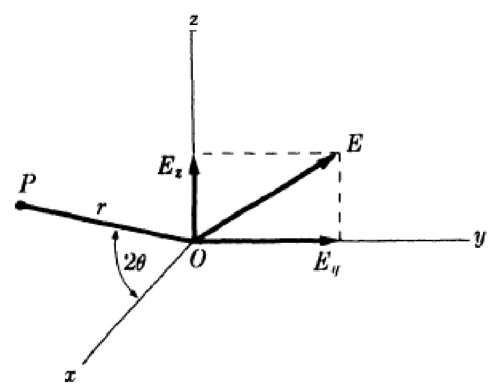
base-centered (left) and body-centered (right) orthorhombic unit cells



Diffraction from the (001) planes of base-centered (left) and body-centered(right) orthorhombic lattices

- Assumption: Bragg law is satisfied for particular value of λ and θ:
- For base-centered (left)**:** Path way ABC between rays 1 and 2 = λ → 1′ and 2′ are in phase→ 001 reflection
- For body-centered (right)**:** Path way DEF between rays 1 and 3 =1/2 λ → 1′ and 3′ are out of phase→ no 001 reflection from body centered lattice

1. Scattering by an electron:



- Thomson equation:

Incident beam direction: ox

Scattering angle: 2θ

Scattered intensity at P in the xz plane depends on the angle of scattering:

$$\boldsymbol{I_P = I_0 \frac{K}{r^2}\left(\frac{1+\cos^2 2\theta}{2}\right)}, K = 7.94 \times 10^{-30}\, m^2$$

$\frac{I_P}{I_0} = 7.94 \times 10^{-26}$ in the forward direction at 1 cm from the electron!

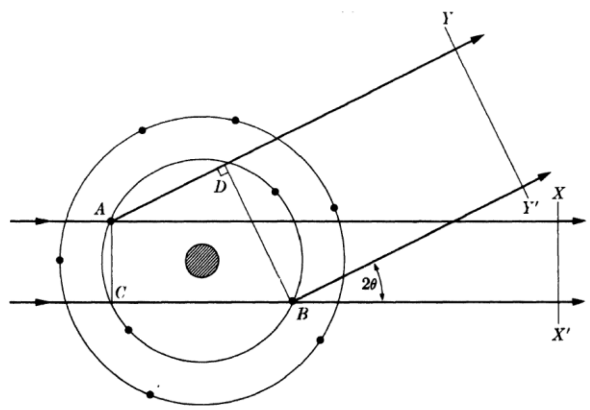
$\frac{1}{2}(1 + cos^2 2\theta)$ is called polarization factor.

- The scattered beam has the same wavelength and frequency as the incident beam and is said to be coherent with it, since there is a definite relationship between the phase of the scattered beam and that of the incident beam which produced it.
- There is another and quite different way in which an electron can scatter x-rays (Compton Effect). This occurs whenever x-rays encounter loosely bound or free electrons and can be understand only by considering the incident beam not as a wave motion, but as a stream of x-ray quanta or photons.

$$\Delta\lambda\,(\text{Å}) = \lambda_2 - \lambda_1 = 0.0486\,sin^2\theta$$

- The scattered radiation→ its phase has no fixed relation to the phase of the incident beam, and cannot produce any interference effects and cannot take part in diffraction, incoherent radiation.

2. Scattering by an atom:



- Electrons at different points in space→ differences in phase
- The scattered wave by electrons A and B: path difference = CB-AD < λ→partial interference → less amplitude than forward case

- Atomic scattering factor (form factor)→ efficiency of scattering in a given direction

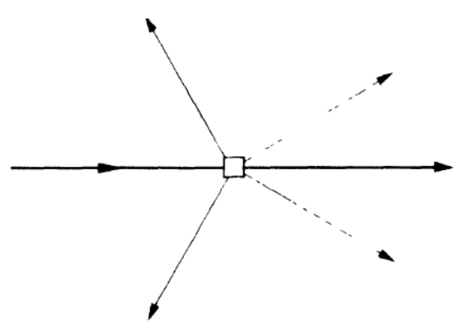
$$f = \frac{amplitude\ of\ the\ wave\ scattered\ by\ an\ atom}{amplitude\ of\ the\ wave\ scattered\ by\ one\ electron}$$

→f = Z for in forward direction!

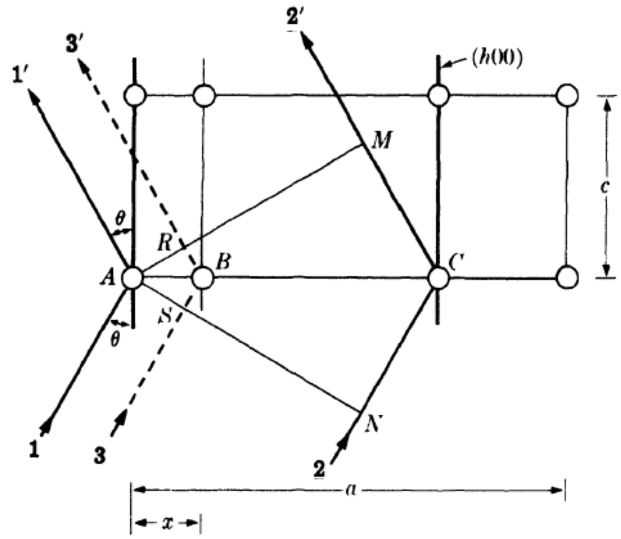
- f depends on scattering angle (θ) and the wavelength (λ)→ f ∝ (sinθ)/λ

- A intensity of the wave ∝ ampiltude^2
  →a scattered intensity from an atom ∝ f^2

3. Scattering by an unit cell



- The atoms are arranged in a periodic fashion in space→scattered radiation is limited to certain directions (Bragg law)
- The wave scattered by individual atoms of a unit cell are not necessarily in phase except in forward direction
- Finding the phase difference between wave scattering by an atom at the origin and other atoms whose position is variable in the x direction only.



Orthorhombic unit cell: A as origin

- Diffraction from (h00) planes→ Path difference between 2' and 1'=MCN=$2d_{h00}\sin\theta = \lambda$, d_{h00}=a/h
- Path difference between 3' and 1' $\delta_{3'1'}$=RBS=(AB/**AC**)λ=(x/**a/h**)λ
- If path difference is δ→ phase difference is **$\phi = (\delta/\lambda)(2\pi)$**

  →$\phi_{3'1'} = (\delta_{3'1'}/\lambda)(2\pi) = 2\pi hx/a$, u=x/a → $\phi_{3'1'} = 2\pi hu$
- Phase difference between the wave scattered by atom B and the scattered by atom A at the origin, for the hkl reflection: ***$\varphi = 2\pi(hu+kv+lw)$*** *where* fractional coordinates of atom B: u=x/a, v=y/b, and w=z/c

  Scattering from a unit cell= adding waves of different phase and amplitude
- We can express any scattered wave in the complex exponential from→**$Ae^{i\phi} = fe^{2\pi i(hu+kv+lw)}$**
- the resultant wave scattered by all the atoms of the unit cell=structure factor(F)

  → $F = f_1e^{2\pi i(hu_1+kv_1+lw_1)} + f_2e^{2\pi i(hu_2+kv_2+lw_2)} + f_3e^{2\pi i(hu_3+kv_3+lw_3)} + \ldots$
- $\boldsymbol{F_{hkl} = \sum_1^N f_n e^{2\pi i(hu_n+kv_n+lw_n)}}$**,** N atoms of the unit cell

$$|F| = \frac{amplitude\ of\ the\ wave\ scattered\ by\ all\ the\ atoms\ of\ a\ unit\ cell}{amplitude\ of\ the\ wave\ scattered\ by\ one\ electron}$$

- The intensity of the beam diffracted by all atoms of unit cell in direction predicted by Bragg law $\propto |F|^2$