

X-ray Diffraction

Interaction of Waves

Reciprocal Lattice and Diffraction

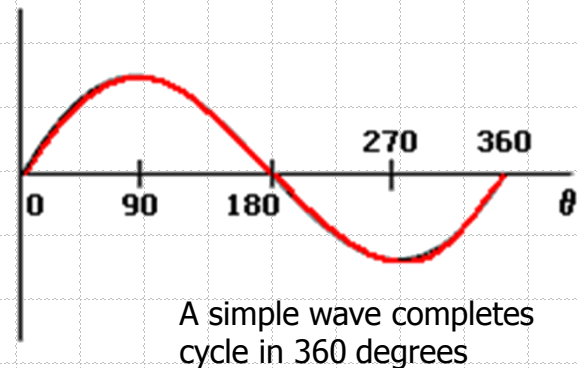
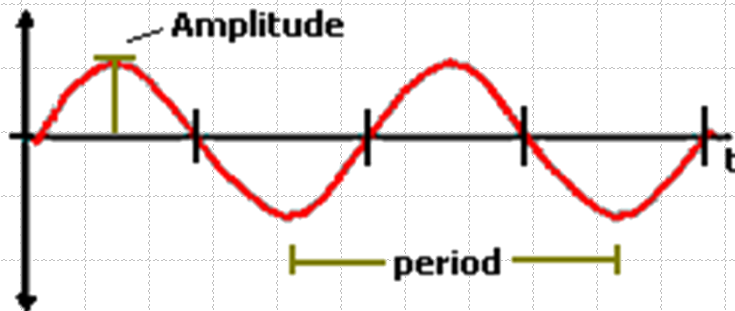
X-ray Scattering by Atoms

The Integrated Intensity

Basic Principles of Interaction of Waves

◆ Periodic waves characteristic:

- Frequency ν : number of waves (cycles) per unit time – $\nu = \text{cycles/time}$.
[ν] = 1/sec = Hz.
- Period T : time required for one complete cycle – $T = 1/\nu = \text{time/cycle}$. [T] = sec.
- Amplitude A : maximum value of the wave during cycle.
- Wavelength λ : the length of one complete cycle. [λ] = m, nm, Å.



$$E(t, x) = A \exp(kx - \omega t)$$
$$= A \exp 2\pi\nu \left(\frac{x}{\lambda} - t \right) = A \exp 2\pi \left(\frac{x}{\lambda} - \nu t \right)$$

$$\omega = 2\pi\nu, \quad k = \frac{2\pi}{\lambda}$$

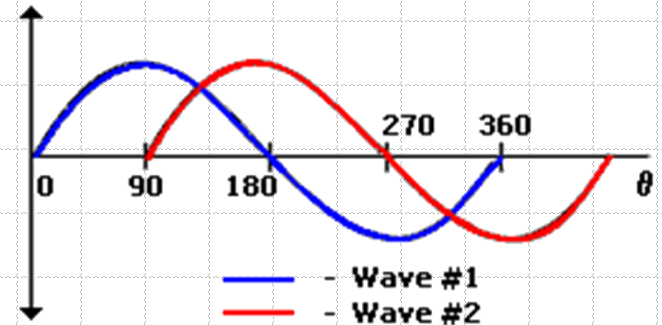
Basic Principles of Interaction of Waves

- ◆ Consider two waves with the same wavelength and amplitude but displaced a distance x_0 .
- ◆ The phase shift:

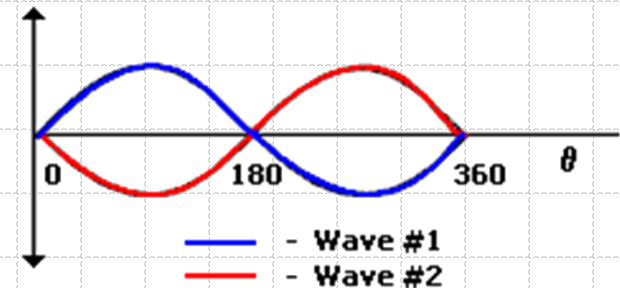
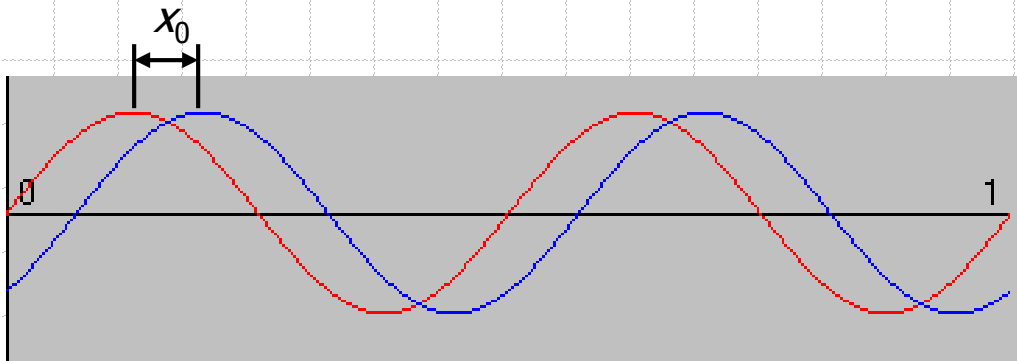
$$\varphi = 2\pi \left(\frac{x_0}{\lambda} \right)$$

$$E_1(t) = A \exp(i\omega t)$$

$$E_2(t) = A \exp(i\omega t + \varphi)$$



Waves #1 and #2 are 90° out of phase

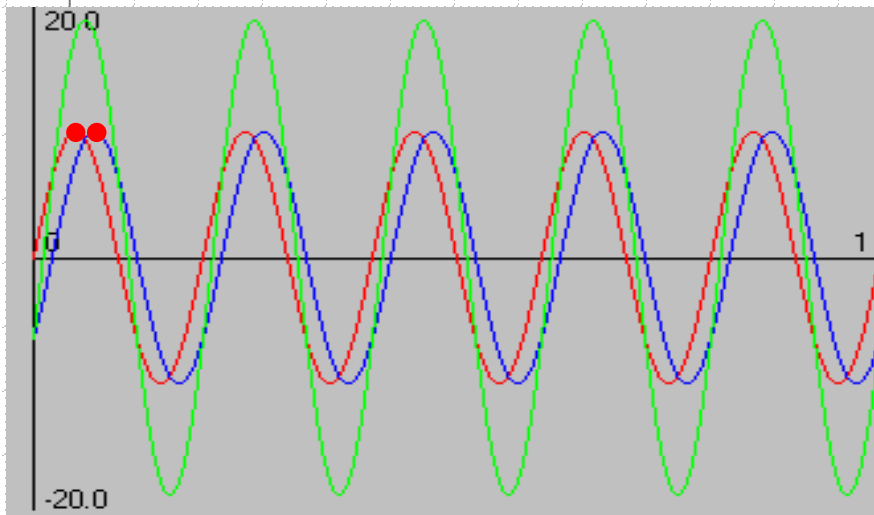


Waves #1 and #2 are 180° out of phase

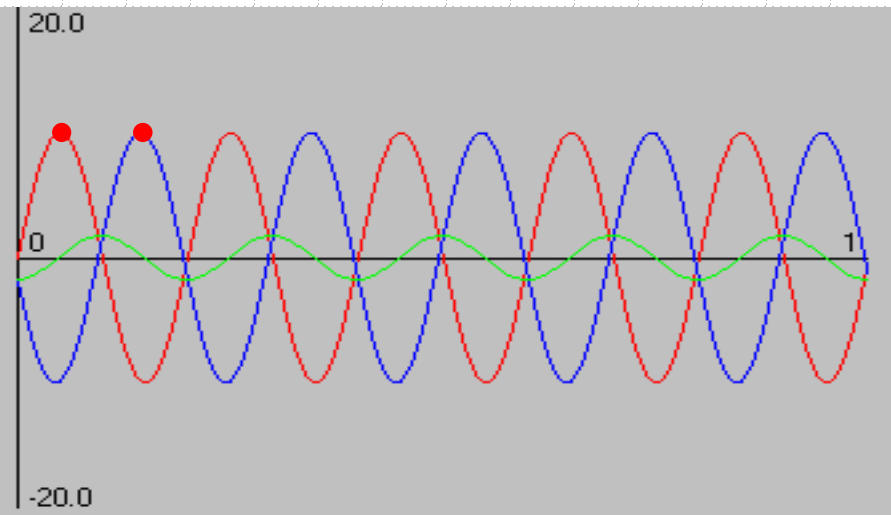
When similar waves combine, the outcome can be constructive or destructive interference

Superposition of Waves

- ◆ Resulting wave is algebraic sum of the amplitudes at each point



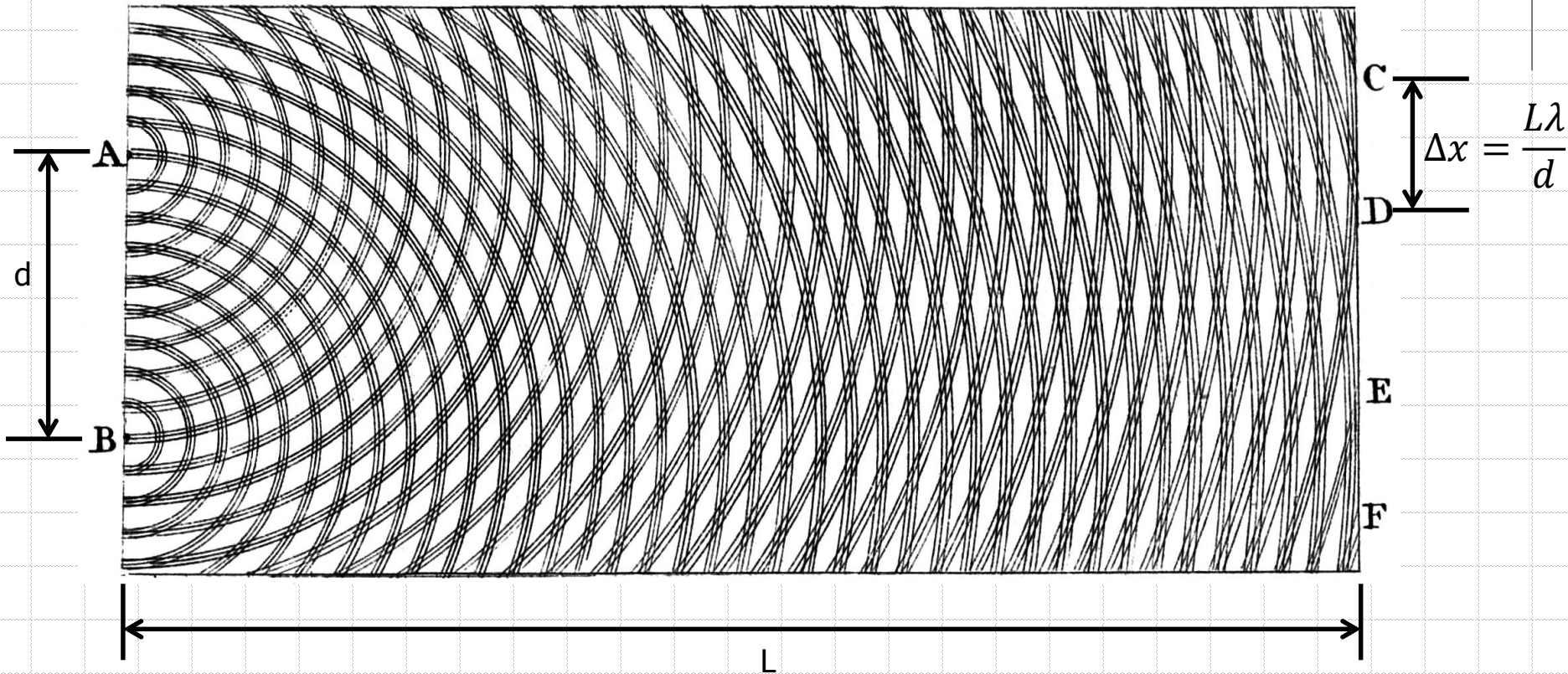
Small difference in phase



Large difference in phase

Superposition of Waves

◆ Thomas Young's diagram of double slit interference (1803)



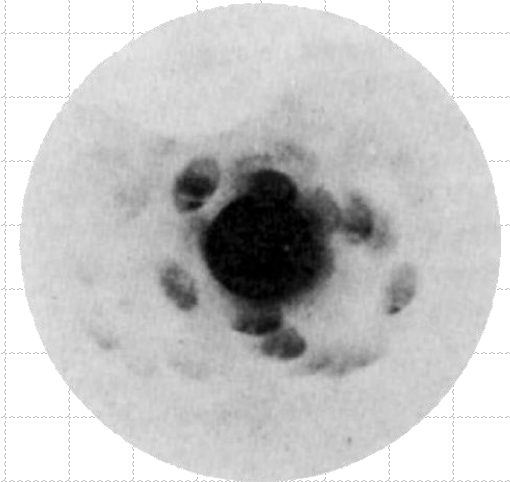
The angular spacing of the fringes is given by $\theta_f \approx \frac{\lambda}{d}$, where $\theta_f \ll 1$

The discovery of X-ray diffraction and its use as a probe of the structure of matter

- The reasoning: x-rays have a wavelength similar to the interatomic distances in crystals, and as a result, the crystal should act as a diffraction grating.
- 1911, von Laue suggested to one of his research assistants, Walter Friedrich, and a doctoral student, Paul Knipping, that they try out x-rays on crystals.
- April 1912, von Laue, Friedrich and Knipping had performed their pioneering experiment on copper sulfate.



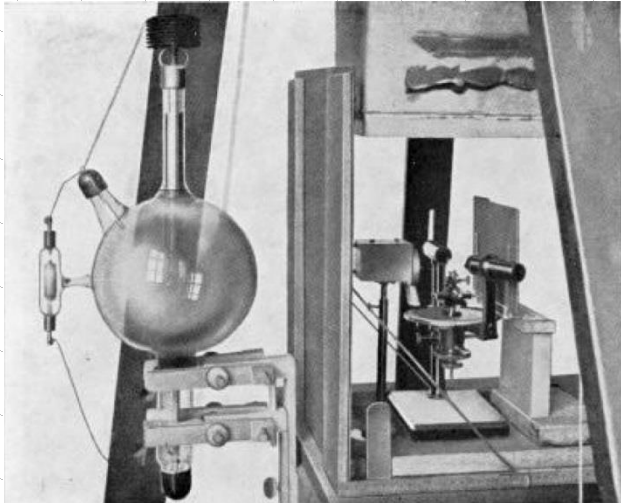
Max von Laue



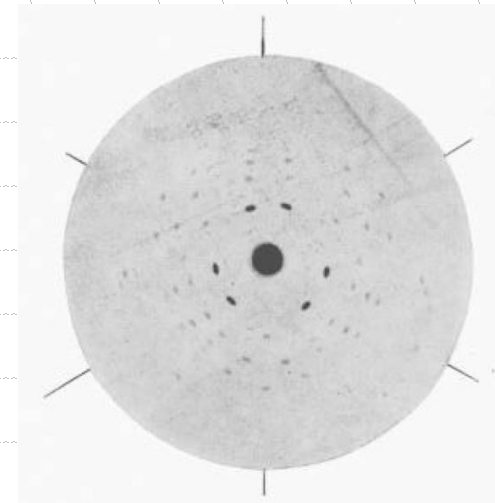
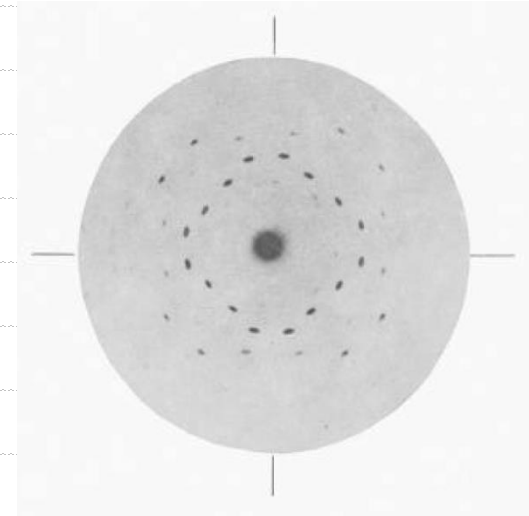
First diffraction pattern from NaCl crystal

The discovery of X-ray diffraction and its use as a probe of the structure of matter

- They found that if the interatomic distances in the crystal are known, then the wavelength of the X-rays can be measured, and alternatively, if the wavelength is known, then X-ray diffraction experiments can be used to determine the interplanar spacings of a crystal.
- The three were awarded Nobel Prizes in Physics for their discoveries.



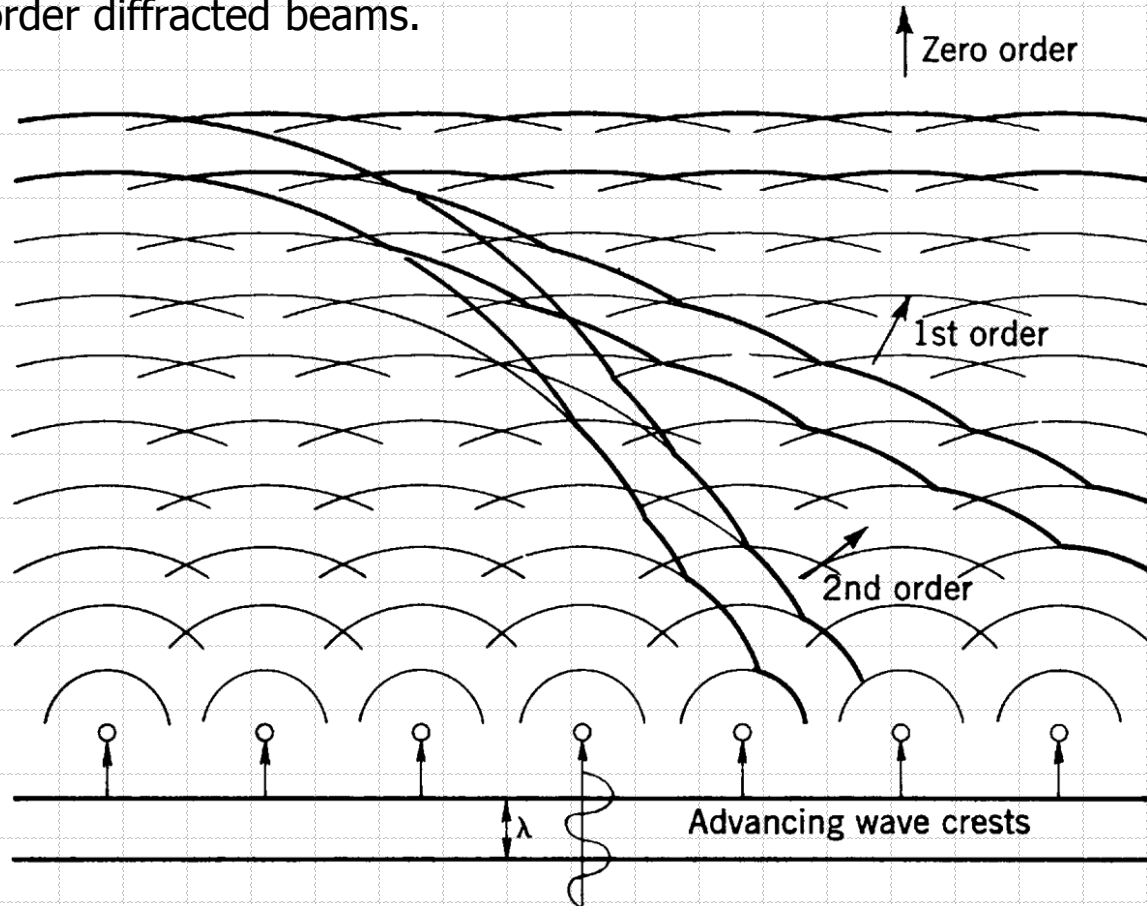
Friedrich & Knipping's improved set-up



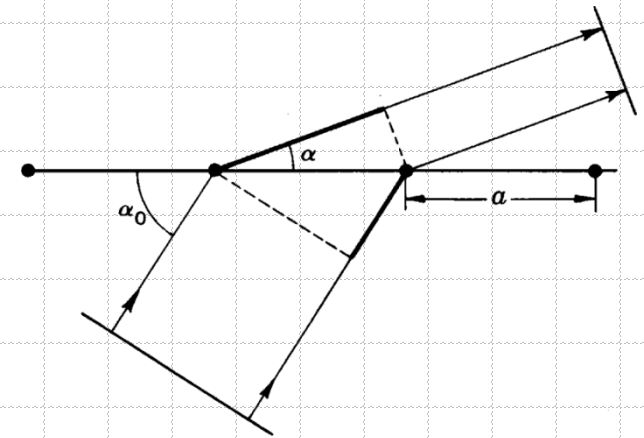
ZnS Laue photographs along four-fold and three-fold axes

The Laue Equations

- ◆ If an X-ray beam impinges on a row of atoms, each atom can serve as a source of scattered X-rays.
- ◆ The scattered X-rays will reinforce in certain directions to produce zero-, first-, and higher-order diffracted beams.



The Laue Equations

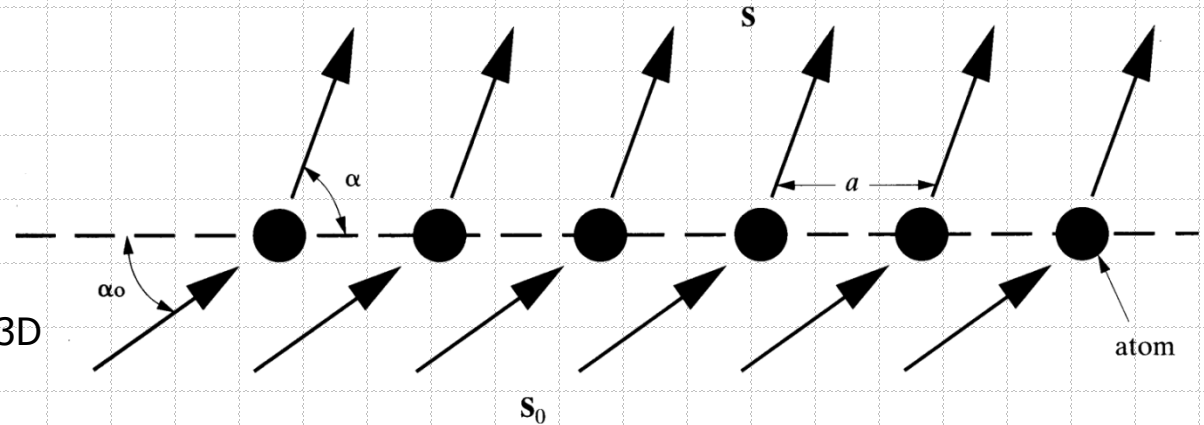


- ◆ Consider 1D array of scatterers spaced a apart.
- ◆ Let x-ray be incident with wavelength λ .

$$a(\cos \alpha - \cos \alpha_0) = h\lambda$$

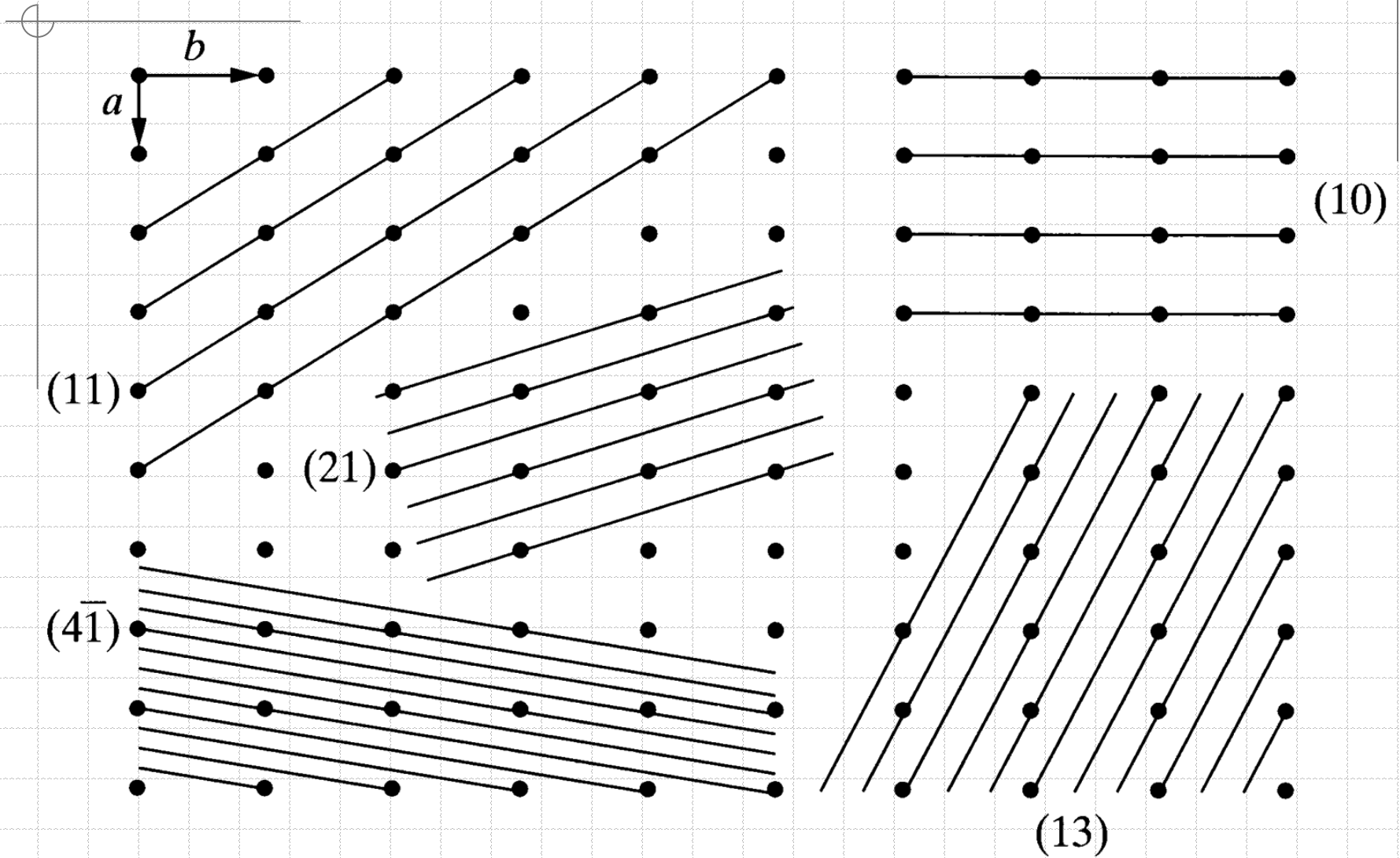
- ◆ In 2D and 3D:

$$\left. \begin{array}{l} a(\cos \alpha - \cos \alpha_0) = h\lambda \\ b(\cos \beta - \cos \beta_0) = k\lambda \\ c(\cos \gamma - \cos \gamma_0) = l\lambda \end{array} \right\} \begin{array}{l} \text{2D} \\ \text{3D} \end{array}$$

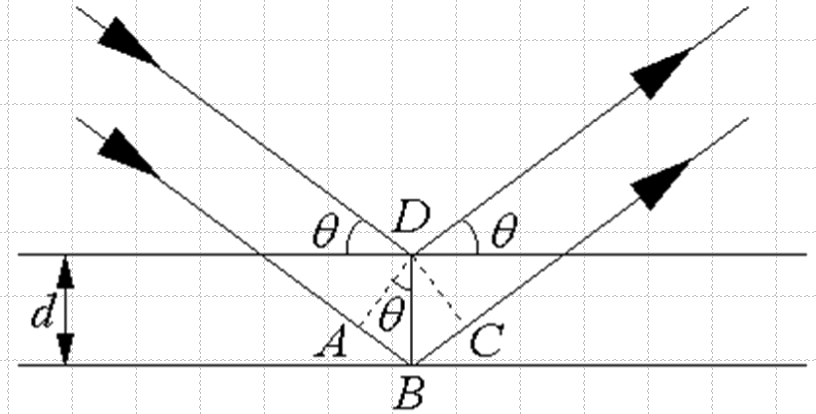
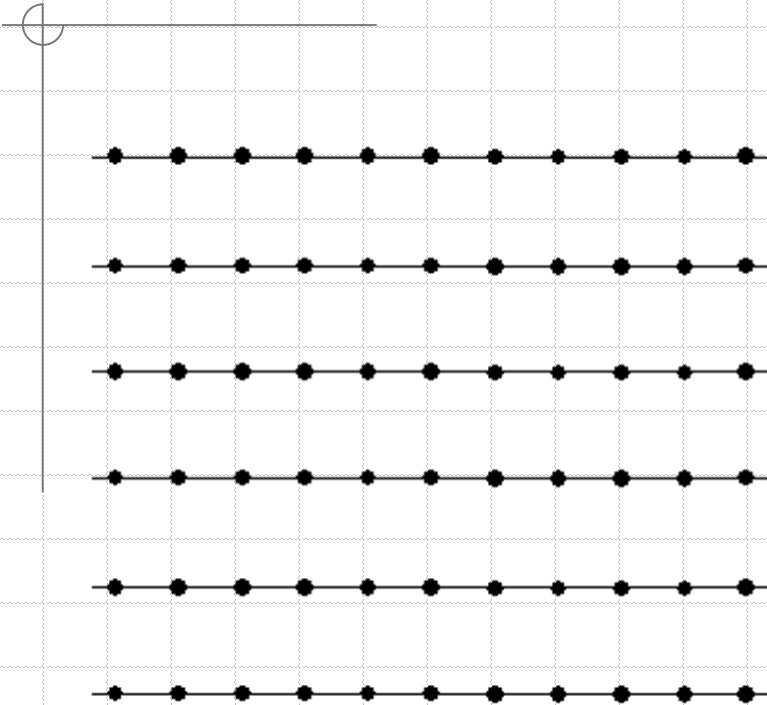


The equations must be satisfied simultaneously, it is in general difficult to produce a diffracted beam with a fixed wavelength and a fixed crystal.

Lattice Planes



Bragg's Law



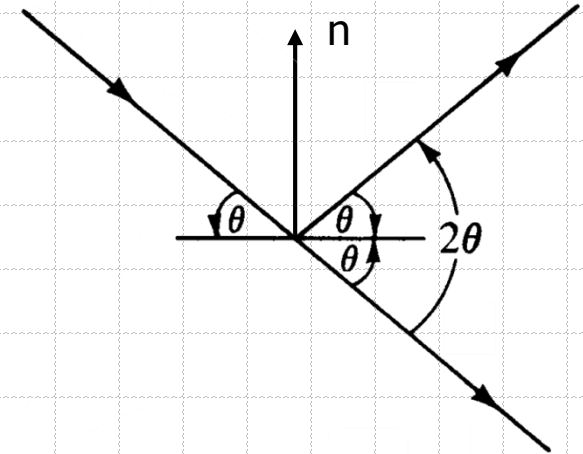
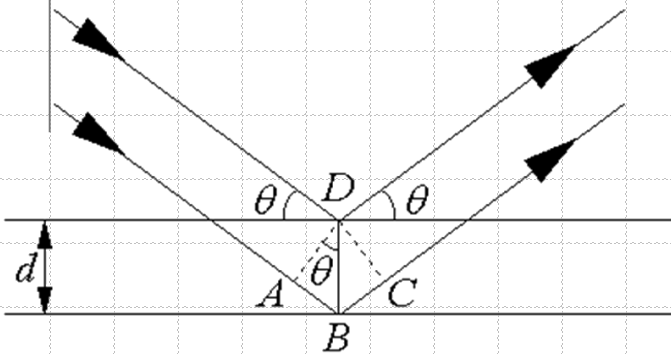
$$AB + BC = 2d \sin \theta$$

Bragg's Law

- ◆ If the path $AB + CD$ is a multiple of the x-ray wavelength λ , then two waves will give a constructive interference:

$$n\lambda = AB + CD = 2d \sin \theta$$

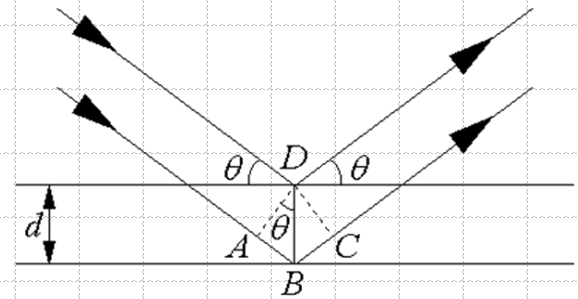
$$2d \sin \theta = n\lambda$$



The diffracted waves will interfere destructively if equation is not satisfied.

Equation is called the Bragg equation and the angle θ is the Bragg angle.

Bragg's Law



- ◆ The incident beam and diffracted beam are always coplanar.
- ◆ The angle between the diffracted beam and the transmitted beam is always 2θ .

Since $\sin\theta \leq 1$: $\frac{n\lambda}{2d} = \sin\theta \leq 1$ For $n = 1$: $\lambda \leq 2d$

For most crystals $d \sim 3 \text{ \AA}$ $\rightarrow \lambda \leq 6 \text{ \AA}$

UV radiation $\lambda \approx 500 \text{ \AA}$
 Cu $K\alpha_1$ $\lambda = 1.5406 \text{ \AA}$

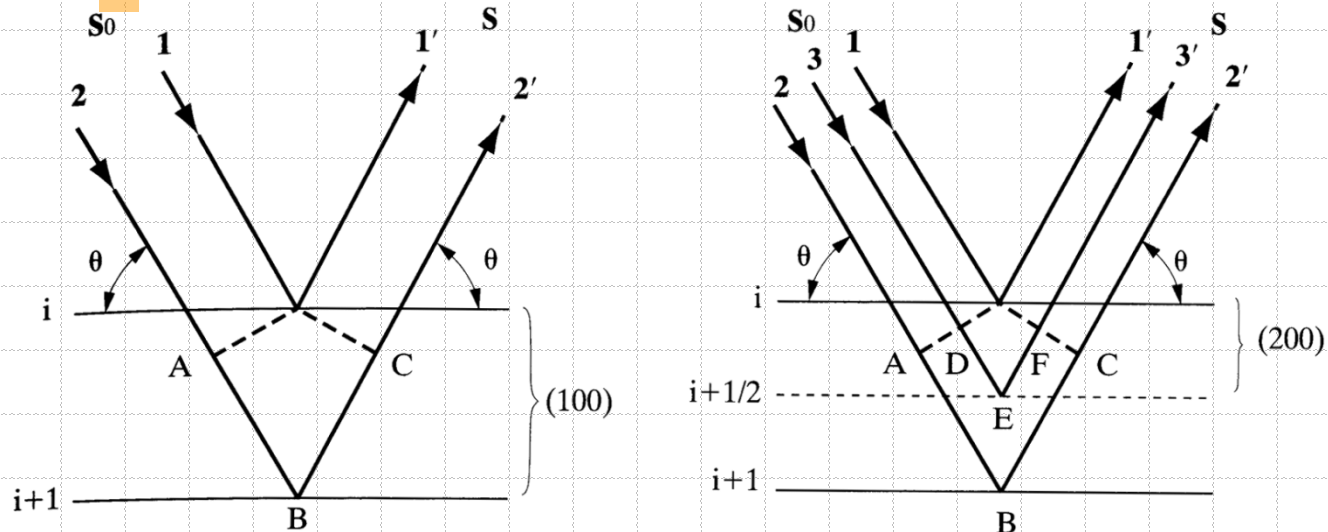
- ◆ Rewrite Bragg's law:

$$\lambda = 2 \frac{d}{n} \sin\theta \rightarrow \lambda = 2d' \sin\theta \rightarrow \underline{\lambda = 2d \sin\theta}$$

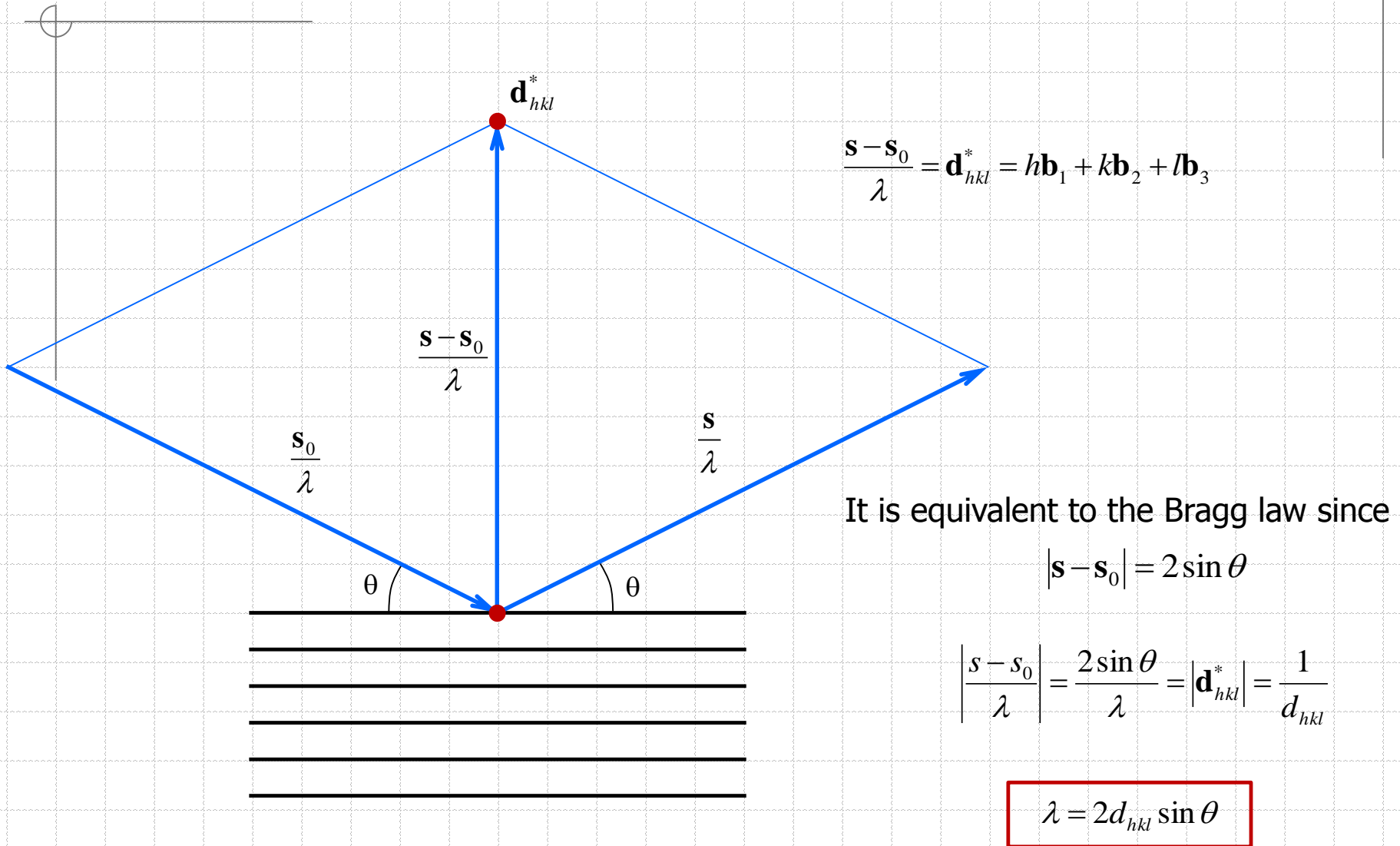
$$\frac{1}{d^2} = \frac{h^2 + k^2 + l^2}{a^2}$$

$$d_{100} = \frac{a}{\sqrt{1^2 + 0 + 0}} = a$$

$$d_{200} = \frac{a}{\sqrt{2^2 + 0 + 0}} = \frac{1}{2}a$$

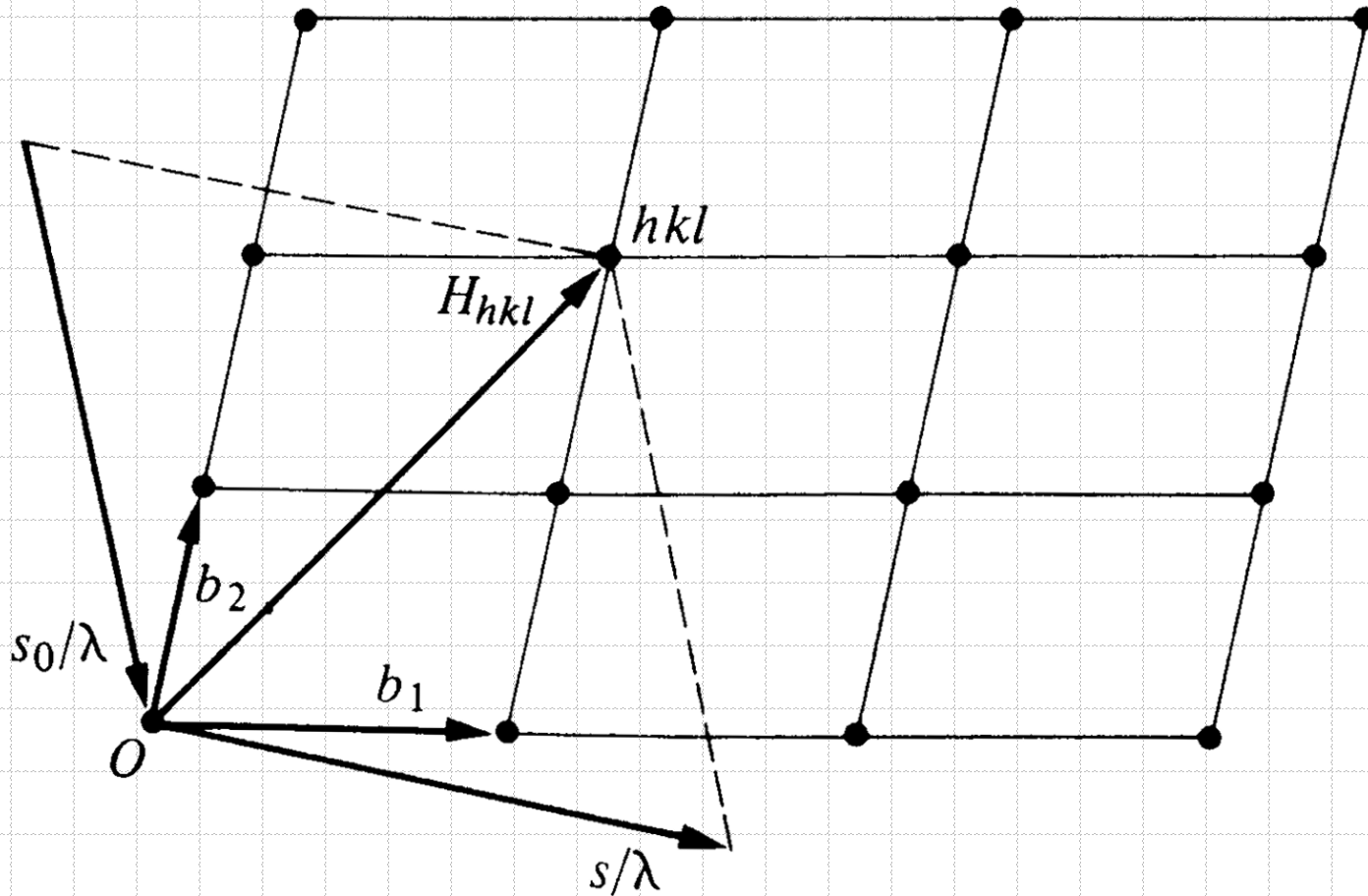


Reciprocal lattice and Diffraction



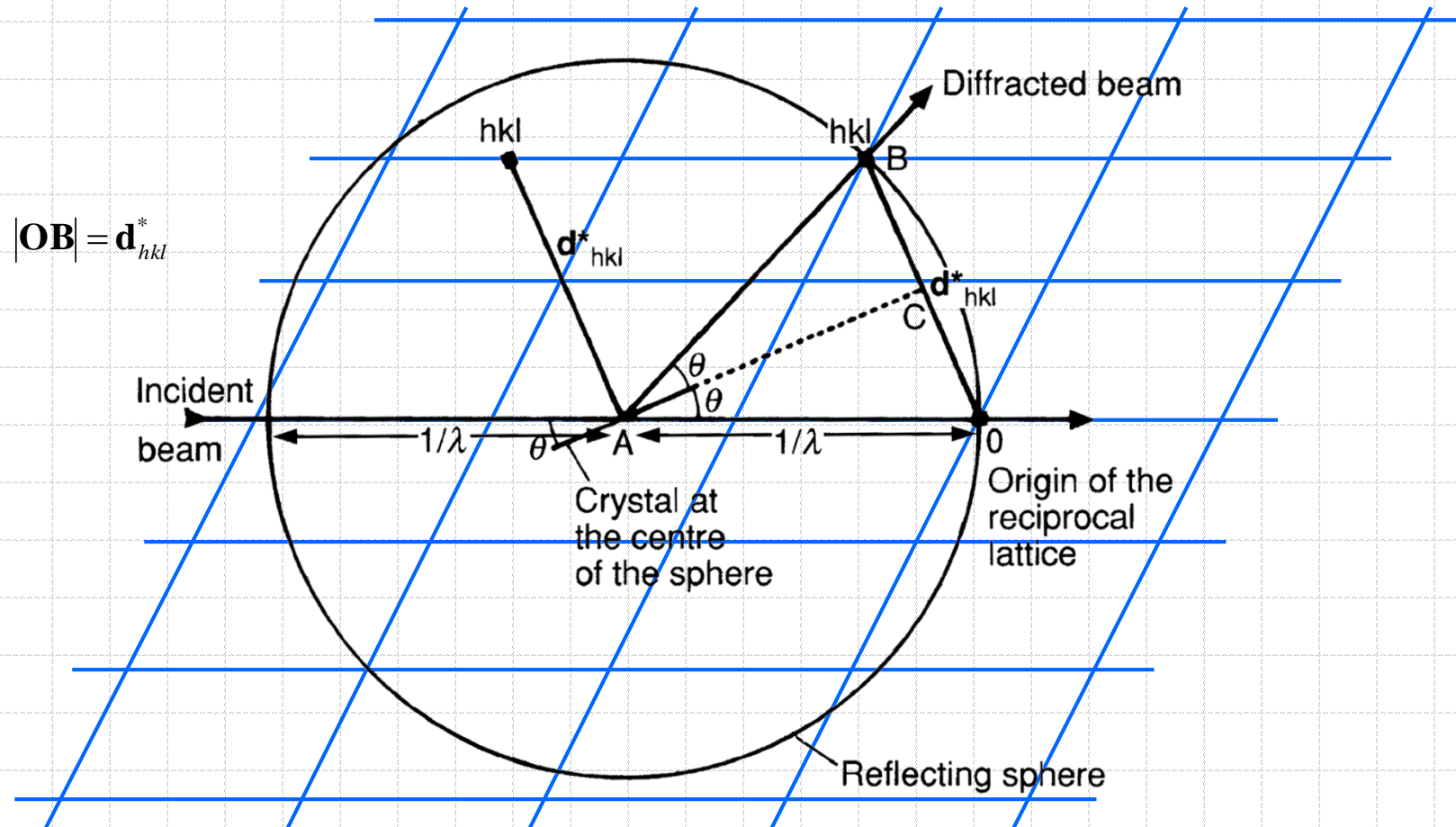
Reciprocal lattice and Diffraction

$$\left| \frac{s - s_0}{\lambda} \right| = \frac{2 \sin \theta}{\lambda} = |\mathbf{d}_{hkl}^*| = \frac{1}{d_{hkl}}$$

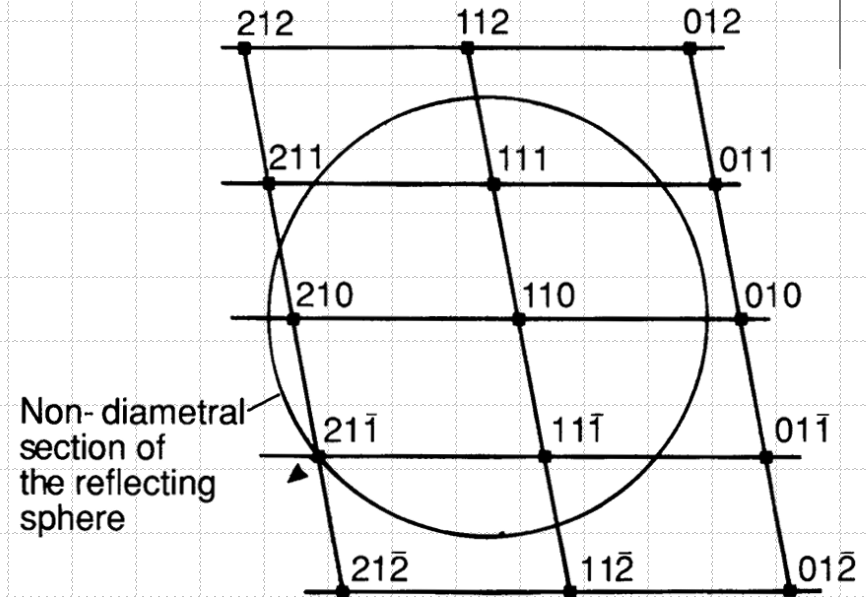
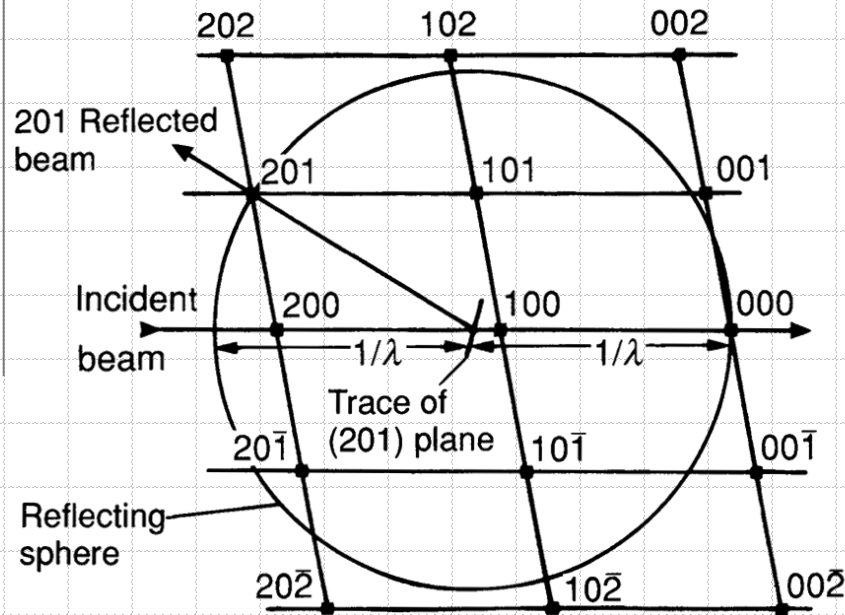


Sphere of Reflection – Ewald Sphere

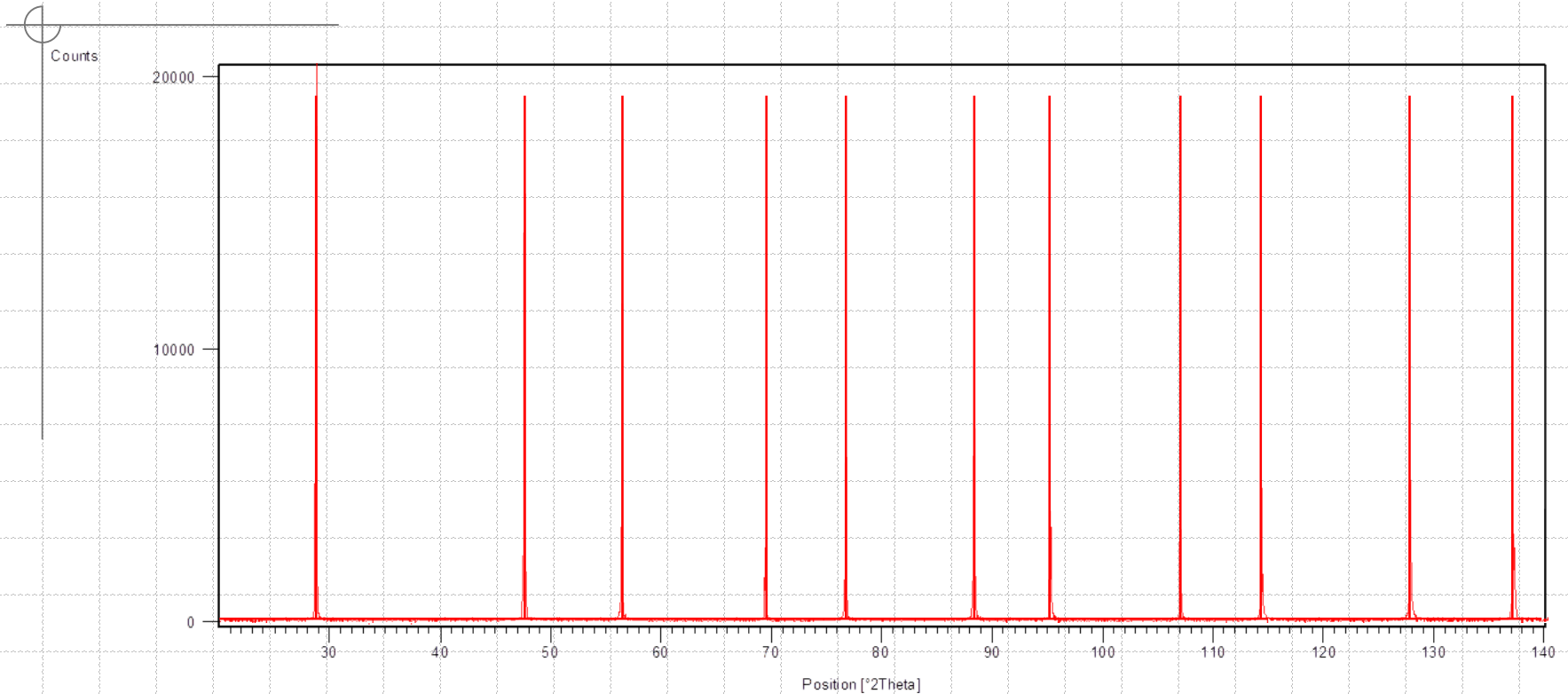
$$|\mathbf{OC}| = \frac{1}{\lambda} \sin \theta = \frac{1}{2} |\mathbf{d}_{hkl}^*| = \frac{1}{2d_{hkl}} \rightarrow \lambda = 2d_{hkl} \sin \theta$$



Sphere of Reflection – Ewald Sphere



Kinematical x-ray diffraction



Silicon lattice constant:
 $a_{\text{Si}} = 5.43 \text{ \AA}$

X-ray wavelength:
 $\lambda = 1.5406 \text{ \AA}$

For cubic crystal:

$$\frac{1}{d^2} = \frac{h^2 + k^2 + l^2}{a^2}$$

Bragg's law:

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

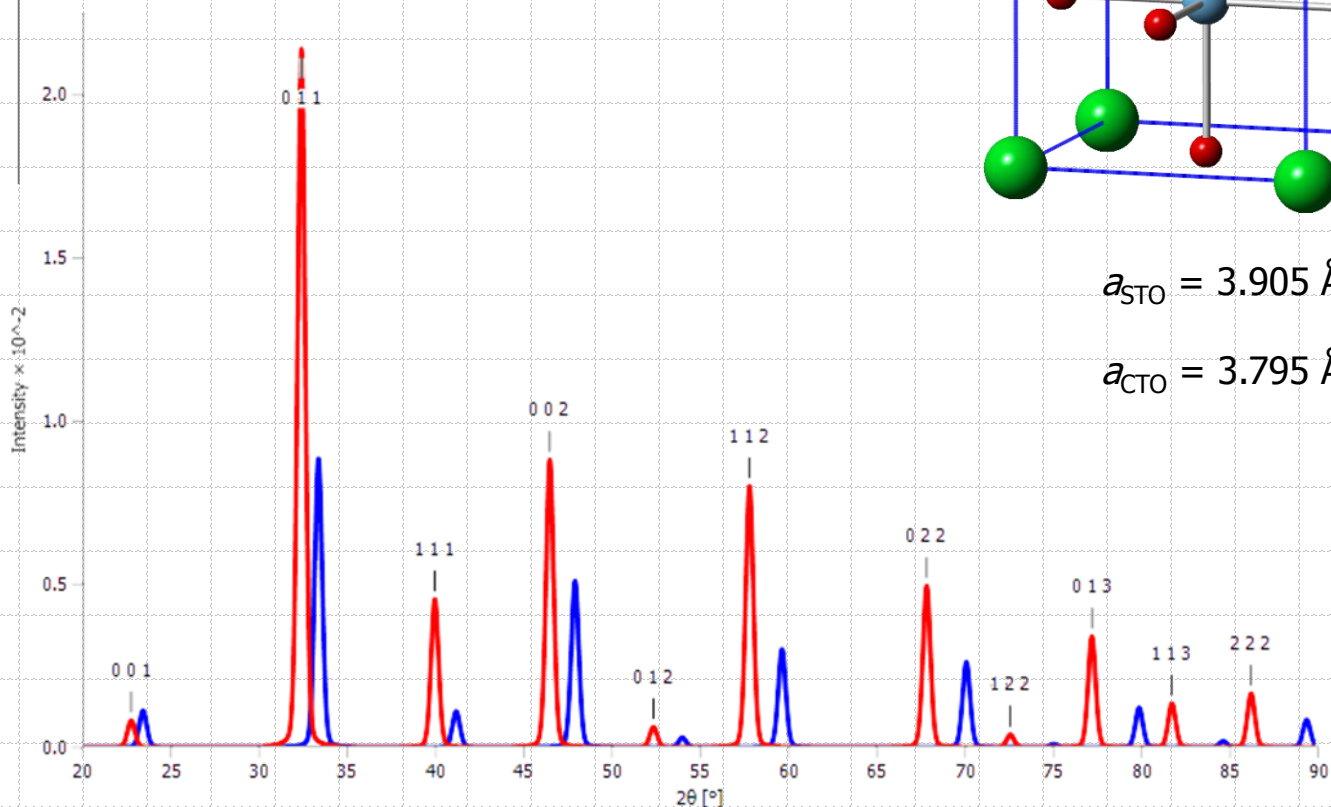
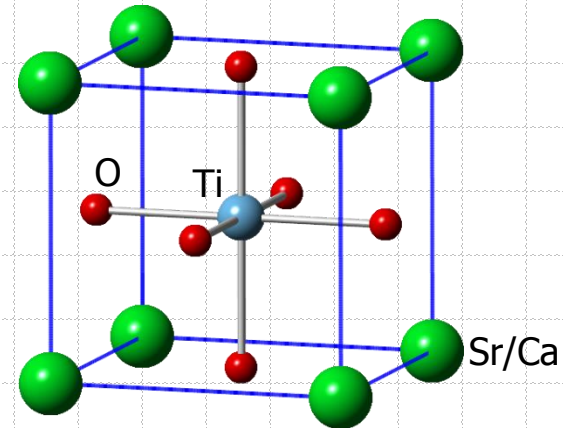
Two perovskites: SrTiO₃ and CaTiO₃

20 ¹S₀
Ca
 Calcium
 40.078
 [Ar]4s²
 6.1132

38 ¹S₀
Sr
 Strontium
 87.62
 [Kr]5s²
 5.6949

Differences:

- Peak position – d-spacing.
- Peak intensity – atom type: **Ca** vs **Sr**.



Scattering by an Electron

- ◆ Elementary scattering unit in an atom is electron
- ◆ Classical scattering by a single free electron – Thomson scattering equation:

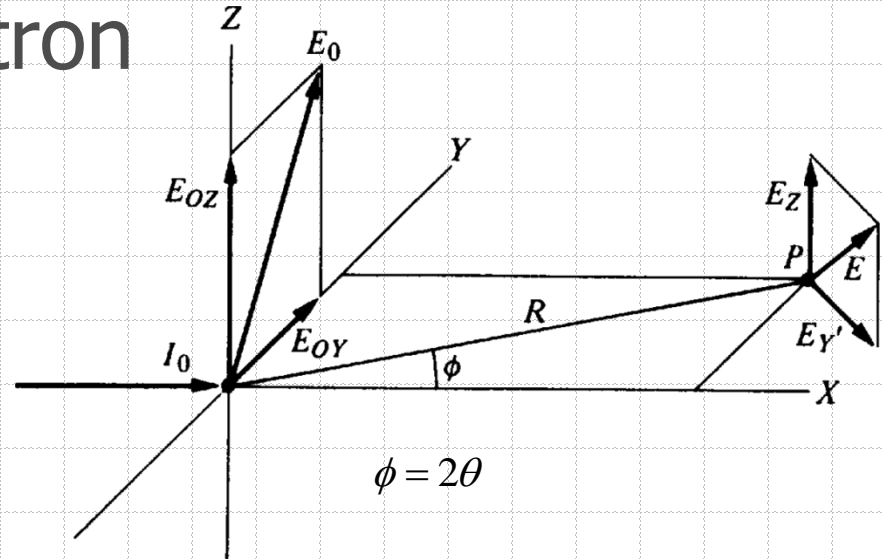
$$I = I_0 \frac{e^4}{m^2 c^4 R^2} \left(\frac{1 + \cos^2 2\theta}{2} \right)$$

The polarization factor of an unpolarized primary beam

$$\frac{e^4}{m^2 c^4} = 7.94 \times 10^{-26} \text{ cm}^2$$

If $R = \text{few cm}$: $\frac{I}{I_0} \approx 10^{-26}$

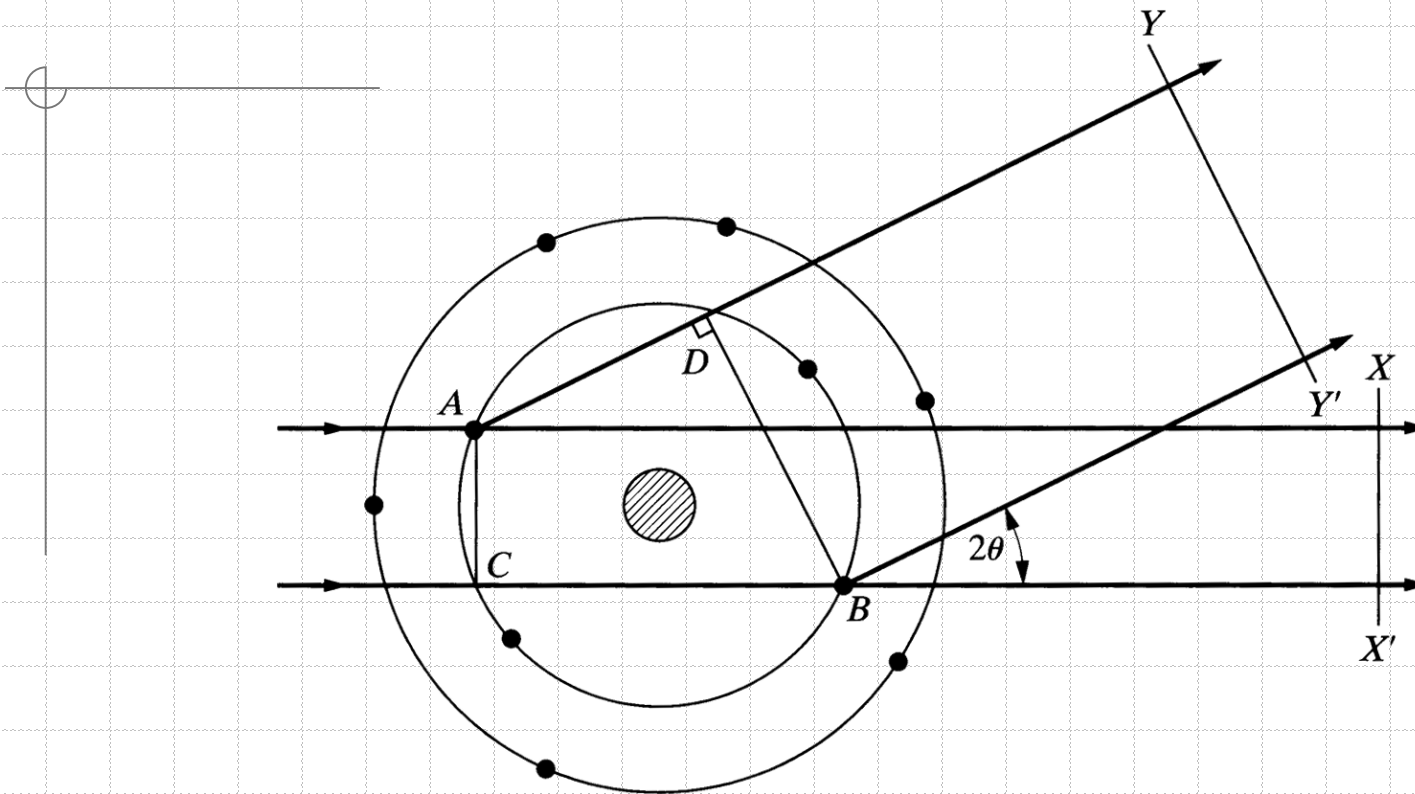
1 mg of matter has $\sim 10^{20}$ electrons



Another way for electron to scatter is manifested in Compton effect.

Cullity p.127

Scattering by an Atom



**Atomic
Scattering
Factor**

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

Scattering by an Atom

◆ Scattering by a group of electrons at positions r_n :

Scattering factor per electron:

$$f_e = \int \exp[(2\pi i / \lambda)(\mathbf{s} - \mathbf{s}_0) \cdot \mathbf{r}] \rho dV$$

Assuming spherical symmetry for the charge distribution $\rho = \rho(r)$ and taking origin at the center of the atom:

$$f_e = \int_0^\infty 4\pi r^2 \rho(r) \frac{\sin kr}{kr} dr$$

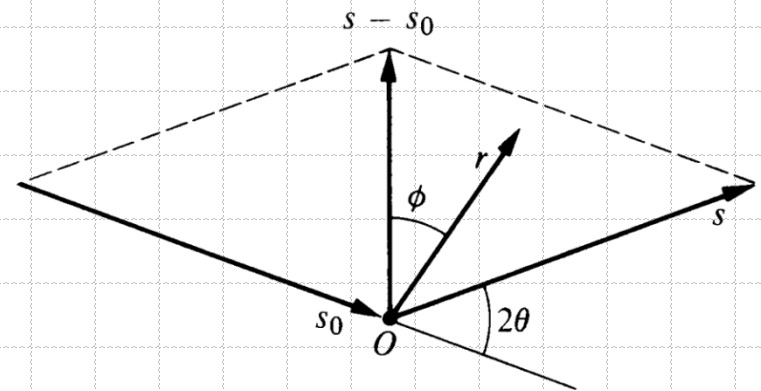
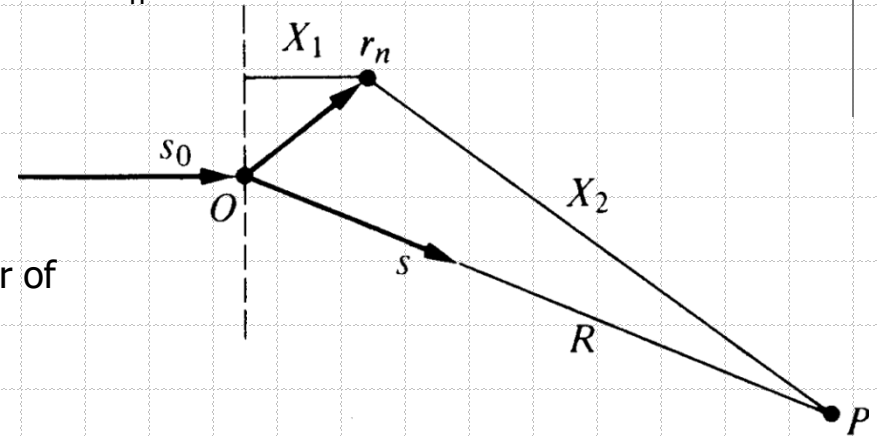
For an atom containing several electrons:

$$f = \sum_n f_{en} = \sum_n \int_0^\infty 4\pi r^2 \rho_n(r) \frac{\sin kr}{kr} dr \quad k = \frac{4\pi \sin \theta}{\lambda}$$

f – atomic scattering factor $f \propto \frac{\sin \theta}{\lambda}$

Calling Z the number of electrons per atom we get:

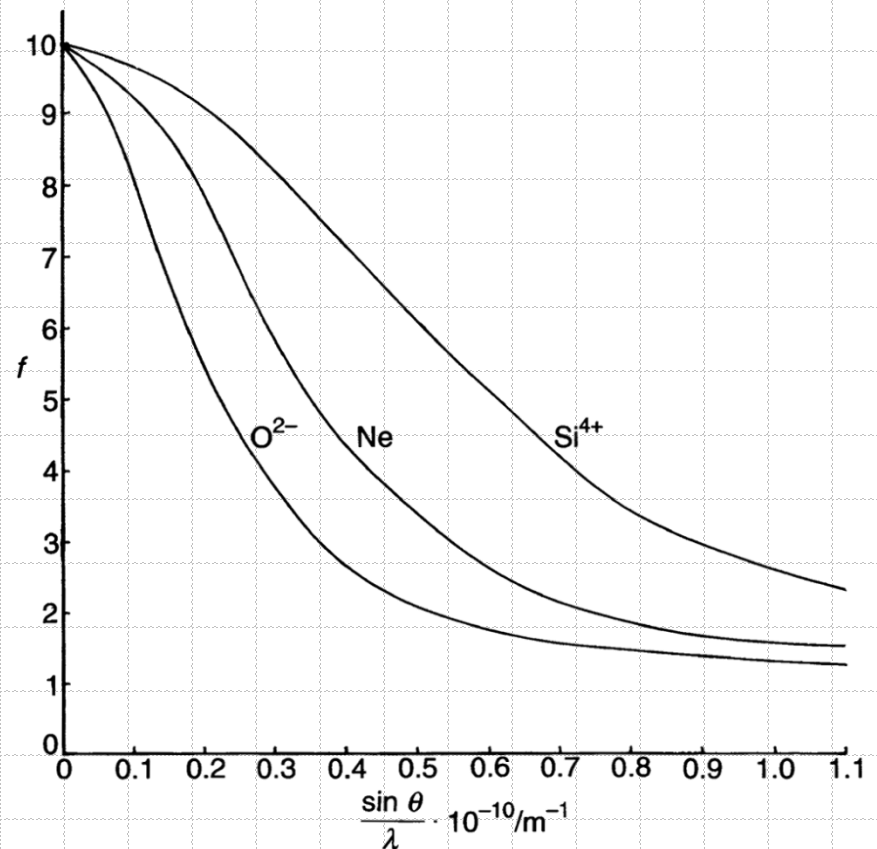
$$\sum_n \int_0^\infty 4\pi r^2 \rho_n(r) dr = Z$$



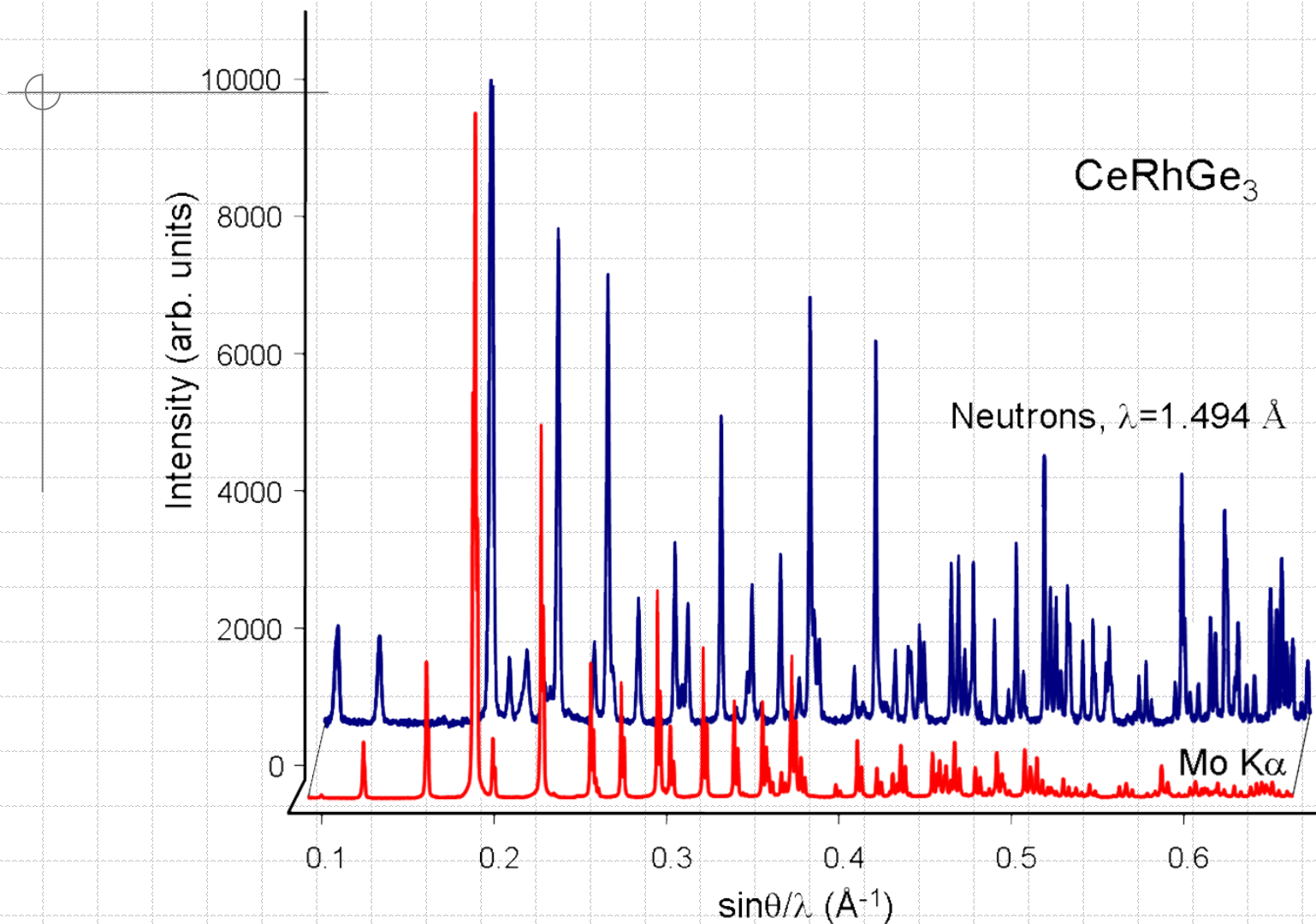
Scattering by an Atom

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

- ◆ The atomic scattering factor $f = Z$ for any atom in the forward direction ($2\theta = 0$):
 $I(2\theta=0) = Z^2$
- ◆ As θ increases f decreases \rightarrow functional dependence of the decrease depends on the details of the distribution of electrons around an atom (sometimes called the form factor)
- ◆ f is calculated using quantum mechanics



Electron vs nuclear density



Powder diffraction patterns collected using Mo $K\alpha$ radiation and neutron diffraction

Scattering by an Atom

Atomic Scattering Factors*

$(\sin \theta)/\lambda(A^{-1})$		0.0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0	1.1	1.2	1.3	1.4	1.5
H	1	1.0	0.81	0.48	0.25	0.13	0.07	0.04	0.02	0.02	0.01	0.01					
He	2	2.0	1.83	1.45	1.06	0.74	0.52	0.36	0.25	0.18	0.13	0.10	0.07	0.05	0.04	0.03	0.03
Li	3	3.0	2.22	1.74	1.51	1.27	1.03	0.82	0.65	0.51	0.40	0.32	0.26	0.21	0.16		
Be	4	4.0	3.07	2.07	1.71	1.53	1.37	1.20	1.03	0.88	0.74	0.62	0.52	0.43	0.37		
B	5	5.0	4.07	2.71	1.99	1.69	1.53	1.41	1.28	1.15	1.02	0.90	0.78	0.68	0.60		
C	6	6.0	5.13	3.58	2.50	1.95	1.69	1.54	1.43	1.32	1.22	1.11	1.01	0.91	0.82	0.74	0.66
N	7	7.0	6.20	4.60	3.24	2.40	1.94	1.70	1.55	1.44	1.35	1.26	1.18	1.08	1.01		
O	8	8.0	7.25	5.63	4.09	3.01	2.34	1.94	1.71	1.57	1.46	1.37	1.30	1.22	1.14		
F	9	9.0	8.29	6.69	5.04	3.76	2.88	2.31	1.96	1.74	1.59	1.48	1.40	1.32	1.25		
Ne	10	10.0	9.36	7.82	6.09	4.62	3.54	2.79	2.30	1.98	1.76	1.61	1.50	1.42	1.35	1.28	1.22
Na	11	11.0	9.76	8.34	6.89	5.47	4.29	3.40	2.76	2.31	2.00	1.78	1.63	1.52	1.44	1.37	1.31
Na ⁺	11	10.0	9.55	8.39	6.93	5.51	4.33	3.42	2.77	2.31	2.00	1.79	1.63	1.52	1.44	1.37	1.30
Mg	12	12.0	10.50	8.75	7.46	6.20	5.01	4.06	3.30	2.72	2.30	2.01	1.81	1.65	1.54		
Al	13	13.0	11.23	9.16	7.88	6.77	5.69	4.71	3.88	3.21	2.71	2.32	2.05	1.83	1.69	1.57	1.48
Si	14	14.0	12.16	9.67	8.22	7.20	6.24	5.31	4.47	3.75	3.16	2.69	2.35	2.07	1.87	1.71	1.60
P	15	15.0	13.17	10.34	8.59	7.54	6.67	5.83	5.02	4.28	3.64	3.11	2.69	2.35	2.10	1.89	1.75
S	16	16.0	14.33	11.21	8.99	7.83	7.05	6.31	5.56	4.82	4.15	3.56	3.07	2.66	2.34		
Cl	17	17.0	15.33	12.00	9.44	8.07	7.29	6.64	5.96	5.27	4.60	4.00	3.47	3.02	2.65		
Cl ⁻	17	18.0	16.02	12.20	9.40	8.03	7.28	6.64	5.97	5.27	4.61	4.00	3.47	3.03	2.65	2.35	2.11
A	18	18.0	16.30	12.93	10.20	8.54	7.56	6.86	6.23	5.61	5.01	4.43	3.90	3.43	3.03		
K	19	19.0	16.73	13.73	10.97	9.05	7.87	7.11	6.51	5.95	5.39	4.84	4.32	3.83	3.40	3.01	2.71
Ca	20	20.0	17.33	14.32	11.71	9.64	8.26	7.38	6.75	6.21	5.70	5.19	4.69	4.21	3.77	3.37	3.03

(cont.)

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Scattering by a Unit Cell

$$F_{hkl} = \frac{\text{amplitude scattered by atoms in unit cell}}{\text{amplitude scattered by single electron}}$$

For atoms A & C

$$\delta_{2'1'} = MCN = 2d_{h00} \sin \theta = \lambda$$

$$d_{h00} = AC = \frac{a}{h}$$

For atoms A & B

$$\delta_{3'1'} = RBS = \frac{AB}{AC} MCN = \frac{AB}{AC} \lambda = \frac{x}{a} \lambda$$

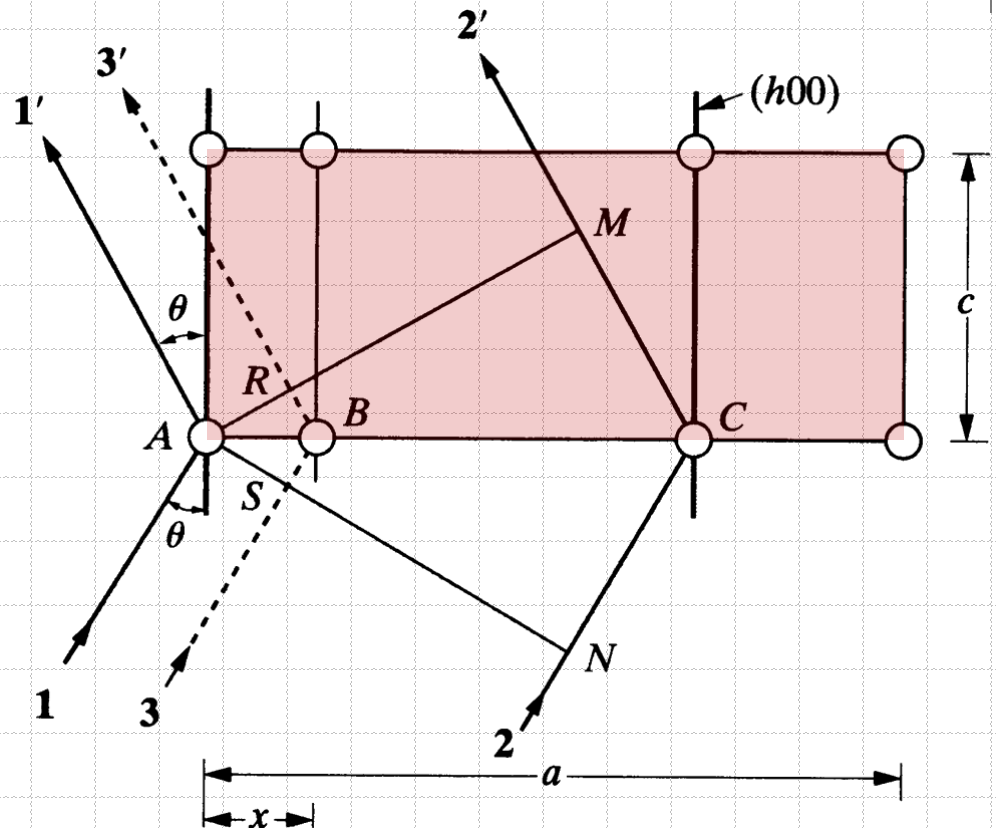
phase $\phi = 2\pi \frac{\delta}{\lambda}$

$$\phi_{3'1'} = 2\pi \frac{\delta_{3'1'}}{\lambda} = \frac{2\pi hx}{a}$$

If atom B position: $u = x/a$

$$\phi_{3'1'} = \frac{2\pi hx}{a} = 2\pi hu$$

For 3D: $\phi = 2\pi(hu + kv + lw)$



Scattering by a Unit Cell

We can write:

$$Ae^{i\phi} = fe^{2\pi i(hu+kv+lw)}$$

$$F = f_1e^{i\phi_1} + f_2e^{i\phi_2} + f_3e^{i\phi_3} + \dots$$

$$F = \sum_1^N f_n e^{i\phi_n} = \sum_1^N f_n e^{2\pi i(hu_n+kv_n+lw_n)}$$

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

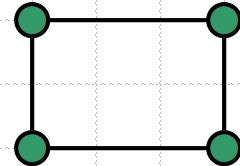
Scattering by a Unit Cell

◆ Examples

Unit cell has one atom at the origin

$$F = fe^{2\pi i0} = f$$

In this case the structure factor is independent of h , k and l ; it will decrease with f as $\sin\theta/\lambda$ increases (higher-order reflections)

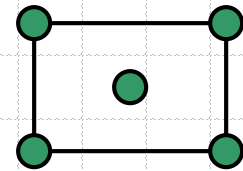


Scattering by a Unit Cell

◆ Examples

Unit cell is base-centered

$$F = fe^{2\pi i 0} + fe^{2\pi i(h/2+k/2)} = f(1 + e^{\pi i(h+k)})$$



$$F = 2f \quad h \text{ and } k \text{ unmixed}$$

$$F = 0 \quad h \text{ and } k \text{ mixed}$$

$$(200), (400), (220) \dots \Rightarrow |F_{hkl}|^2 = 4f^2$$

$$(100), (121), (300) \dots \Rightarrow |F_{hkl}|^2 = 0 \quad \leftarrow \text{“forbidden” reflections}$$

Body-Centered Unit Cell

Examples

For body-centered cell

$$F = fe^{2\pi i(h0+k0+l0)} + fe^{2\pi i(h/2+k/2+l/2)} = f(1 + e^{\pi i(h+k+l)})$$

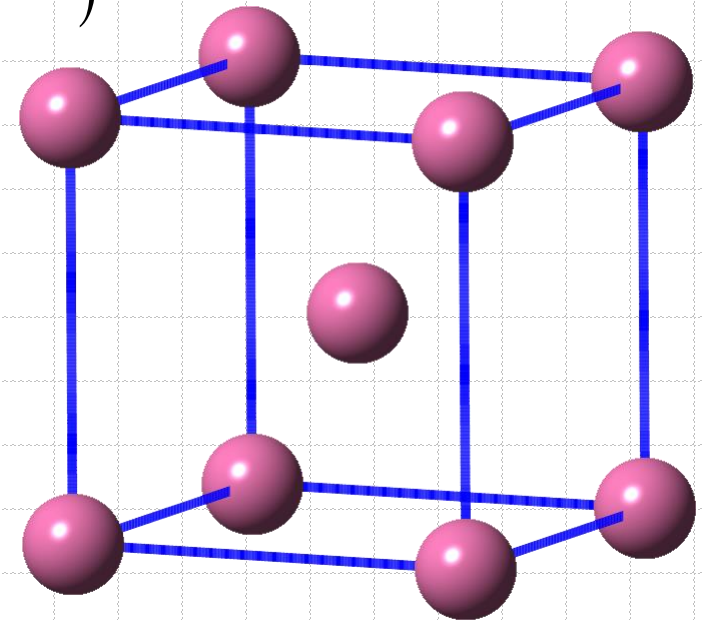
$$F = 2f \quad \text{when } (h + k + l) \text{ is even}$$

$$F = 0 \quad \text{when } (h + k + l) \text{ is odd}$$

$$(200), (400), (220) \dots \Rightarrow |F_{hkl}|^2 = 4f^2$$

$$(100), (111), (300) \dots \Rightarrow |F_{hkl}|^2 = 0$$

← "forbidden" reflections



Body-Centered Unit Cell

Examples

For body centered cell with different atoms:

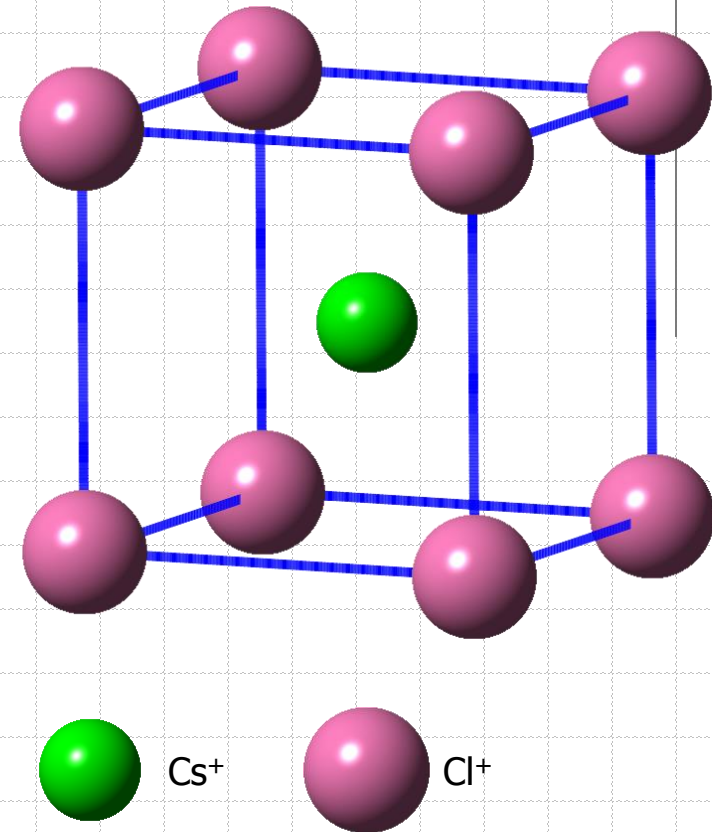
$$F = f_{Cl} e^{2\pi i(h0+k0+l0)} + f_{Cs} e^{2\pi i(h/2+k/2+l/2)}$$
$$= f_{Cl} + f_{Cs} e^{\pi i(h+k+l)}$$

$$F = f_{Cl} + f_{Cs} \quad \text{when } (h + k + l) \text{ is even}$$

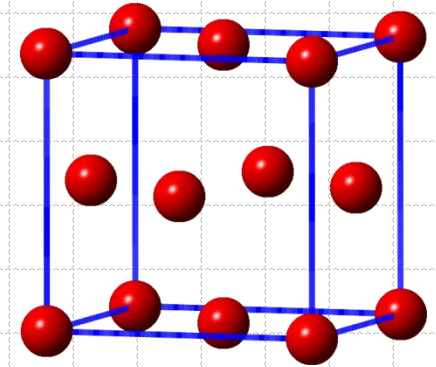
$$F = f_{Cl} - f_{Cs} \quad \text{when } (h + k + l) \text{ is odd}$$

$$(200), (400), (220) \dots \Rightarrow |F_{hkl}|^2 = (f_{Cs} + f_{Cl})^2$$

$$(100), (111), (300) \dots \Rightarrow |F_{hkl}|^2 = (f_{Cs} - f_{Cl})^2$$



Face Centered Unit cell



- ◆ The fcc crystal structure has atoms at 000 , $\frac{1}{2}\frac{1}{2}0$, $\frac{1}{2}0\frac{1}{2}$ and $0\frac{1}{2}\frac{1}{2}$:

$$F_{hkl} = \sum_1^N f_n e^{2\pi i(hu_n + kv_n + lw_n)} = f(1 + e^{\pi i(h+k)} + e^{\pi i(h+l)} + e^{\pi i(k+l)})$$

- ◆ If h , k and l are all even or all odd numbers ("unmixed"), then the exponential terms all equal to $+1 \Rightarrow F = 4f$
- ◆ If h , k and l are mixed even and odd, then two of the exponential terms will equal -1 while one will equal $+1 \Rightarrow F = 0$

$$|F_{hkl}|^2 = \begin{cases} 16f^2, & h, k \text{ and } l \text{ unmixed even and odd} \\ 0, & h, k \text{ and } l \text{ mixed even and odd} \end{cases}$$

The Structure Factor

$$F_{hkl} = \sum_1^N f_n e^{2\pi i(hu_n + kv_n + lw_n)}$$

$$F_{hkl} = \frac{\text{amplitude scattered by all atoms in a unit cell}}{\text{amplitude scattered by a single electron}}$$

- ◆ The structure factor contains the information regarding the types (f) and locations (u, v, w) of atoms within a unit cell
- ◆ A comparison of the observed and calculated structure factors is a common goal of X-ray structural analyses
- ◆ The observed intensities must be corrected for experimental and geometric effects before these analyses can be performed

Integrated Intensity

Peak intensity depends on

- ◆ Structural factors: determined by crystal structure
- ◆ Specimen factors: shape, size, grain size and distribution, microstructure
- ◆ Instrumental factors: radiation properties, focusing geometry, type of detector

We can say that: $I(q) \propto |F(q)|^2$

Integrated Intensity

$$I_{hkl}(q) = K \times p_{hkl} \times L \times P \times A \times T \times E_{hkl} \times |F(q)|^2$$

K – scale factor, required to normalize calculated and measured intensities.

p_{hkl} – multiplicity factor. Accounts for the presence of symmetrically equivalent points in reciprocal lattice.

L – Lorentz multiplier, defined by diffraction geometry.

P – polarization factor. Account for partial polarization of electromagnetic wave.

A – absorption multiplier. Accounts for incident and diffracted beam absorption.

T_{hkl} – preferred orientation factor. Accounts for deviation from complete random grain distribution.

E_{hkl} – extinction multiplier. Accounts for deviation from kinematical diffraction model.

F_{hkl} – the structure factor. Defined by crystal structure of the material

The Multiplicity Factor

- ◆ The multiplicity factor arises from the fact that in general there will be several sets of hkl -planes having different orientations in a crystal but with the same d and F^2 values
- ◆ Evaluated by finding the number of variations in position and sign in $\pm h$, $\pm k$ and $\pm l$ and have planes with the same d and F^2
- ◆ The value depends on hkl and crystal symmetry
- ◆ For the highest cubic symmetry we have:

$100, \bar{1}00, 010, 0\bar{1}0, 001, 00\bar{1}$

$$\rho_{100} = 6$$

$110, \bar{1}\bar{1}0, 1\bar{1}0, \bar{1}\bar{1}0, 101, 10\bar{1}, \bar{1}0\bar{1}, \bar{1}01, 011, 0\bar{1}1, 01\bar{1}, 0\bar{1}\bar{1}$

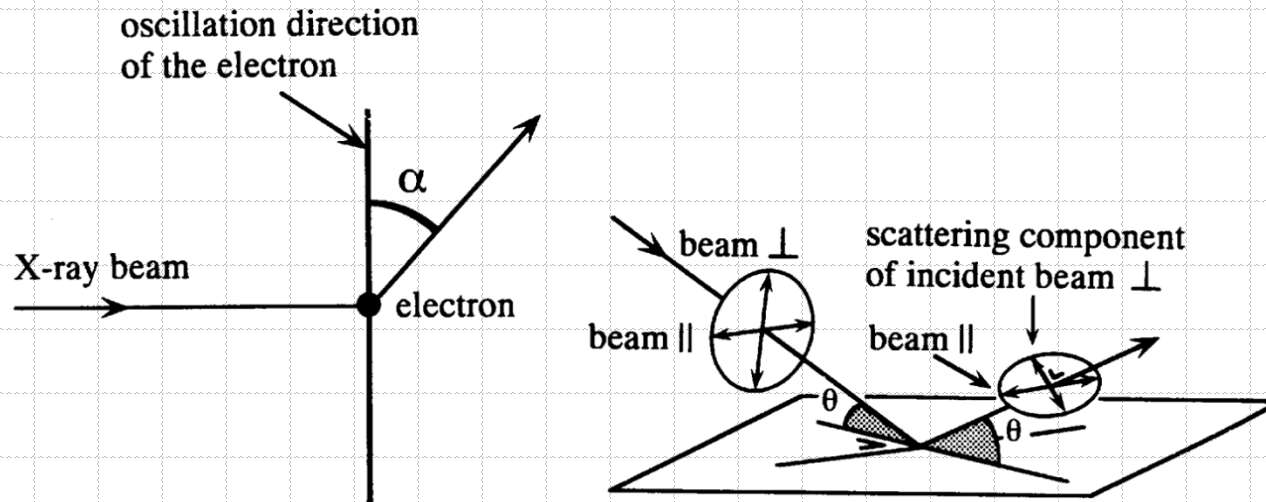
$$\rho_{110} = 12$$

$111, 11\bar{1}, 1\bar{1}\bar{1}, \bar{1}\bar{1}\bar{1}, 1\bar{1}\bar{1}, \bar{1}\bar{1}\bar{1}, \bar{1}\bar{1}\bar{1}, \bar{1}\bar{1}\bar{1}$

$$\rho_{111} = 8$$

The Polarization Factor

- ◆ The polarization factor p arises from the fact that an electron does not scatter along its direction of vibration
- ◆ In other directions electrons radiate with an intensity proportional to $(\sin \alpha)^2$:



The polarization factor (assuming that the incident beam is unpolarized):

$$P = \frac{1 + \cos^2 2\theta}{2}$$

The Lorentz-Polarization Factor

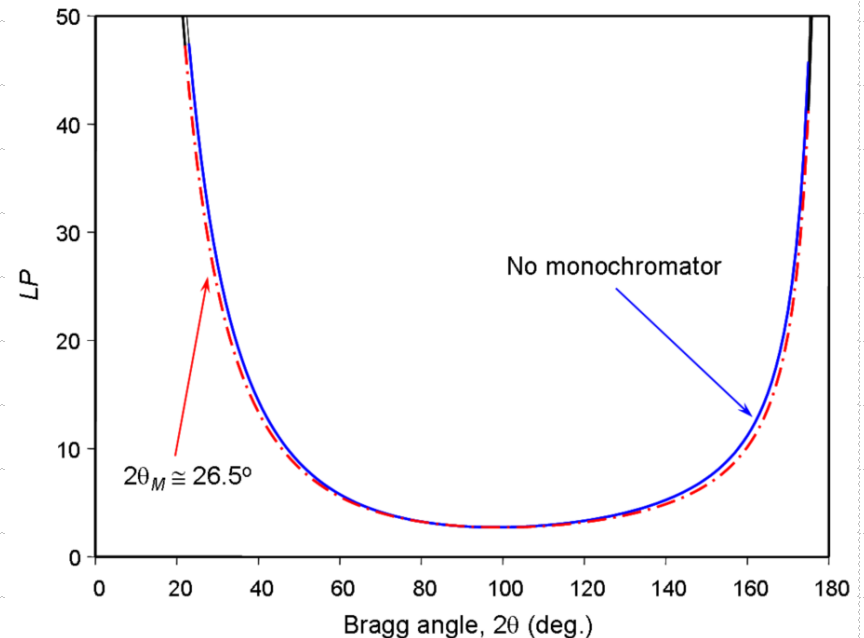
- ◆ The Lorentz factor L depends on the measurement technique used and, for the diffractometer data obtained by the usual θ - 2θ or ω - 2θ scans, it can be written as

$$L = \frac{1}{\sin \theta \sin 2\theta} = \frac{1}{\cos \theta \sin^2 \theta}$$

- ◆ The combination of geometric corrections are lumped together into a single Lorentz-polarization (LP) factor:

$$LP = \frac{1 + \cos^2 2\theta}{\cos \theta \sin^2 \theta}$$

The effect of the LP factor is to decrease the intensity at intermediate angles and increase the intensity in the forward and backwards directions



The Absorption Factor

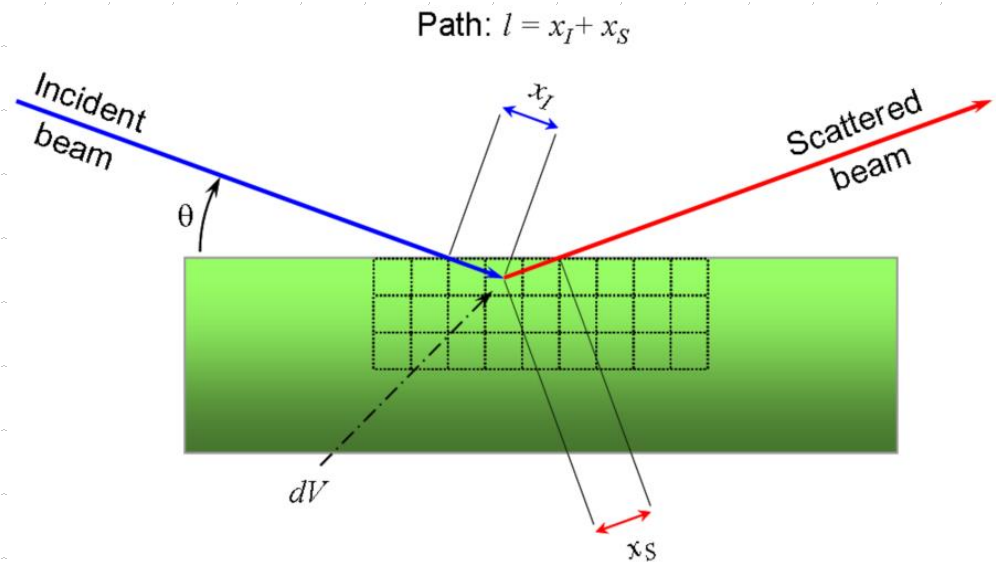
- ◆ Angle-dependent absorption within the sample itself will modify the observed intensity

- Absorption factor for infinite thickness specimen is:

$$A = \frac{\mu}{2}$$

- Absorption factor for thin specimens is given by:

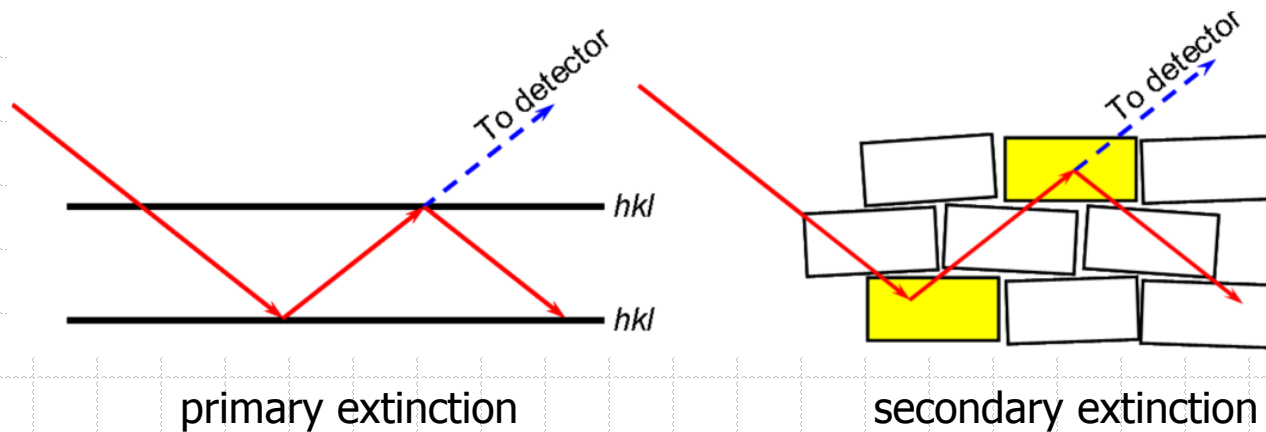
$$A = 1 - \exp\left(-\frac{2\mu t}{\sin \theta}\right)$$



where μ is the absorption coefficient, t is the total thickness of the film

The Extinction Factor

- ◆ Extinction lowers the observed intensity of very strong reflections from perfect crystals



In powder diffraction usually this factor is smaller than experimental errors and therefore neglected

The Temperature Factor

- ◆ As atoms vibrate about their equilibrium positions in a crystal, the electron density is spread out over a larger volume
- ◆ This causes the atomic scattering factor to decrease with $\sin\theta/\lambda$ (or $|S| = 4\pi\sin\theta/\lambda$) more rapidly than it would normally:

The temperature factor is given by:

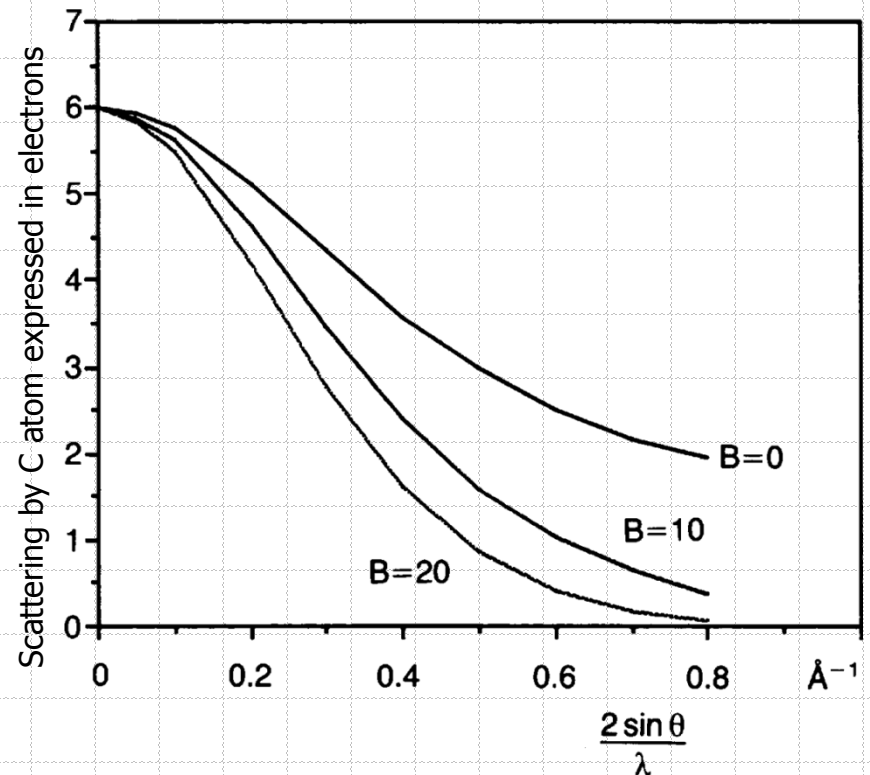
$$e^{-B \frac{\sin^2 \theta}{\lambda^2}}$$

where the thermal factor B is related to the mean square displacement of the atomic vibration:

$$B = 8\pi^2 \times \overline{u^2}$$

This is incorporated into the atomic scattering factor:

$$f \rightarrow f_0 e^{-M} \Rightarrow f^2 \sim e^{-2M}$$



Diffracted Beam Intensity

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

$$I_C(q) = KAp(LP)|F(q)|^2 + I_b$$

where K is the scaling factor, I_b is the background intensity, $q = 4\sin\theta/\lambda$ is the scattering vector for x-rays of wavelength λ

For thin films:

$$I_C(q) = K \left[1 - \exp\left(-\frac{2\mu t}{\sin\theta}\right) \right] \frac{1 + \cos^2 2\theta}{\cos\theta \sin^2\theta} |F(q)|^2 + I_b$$