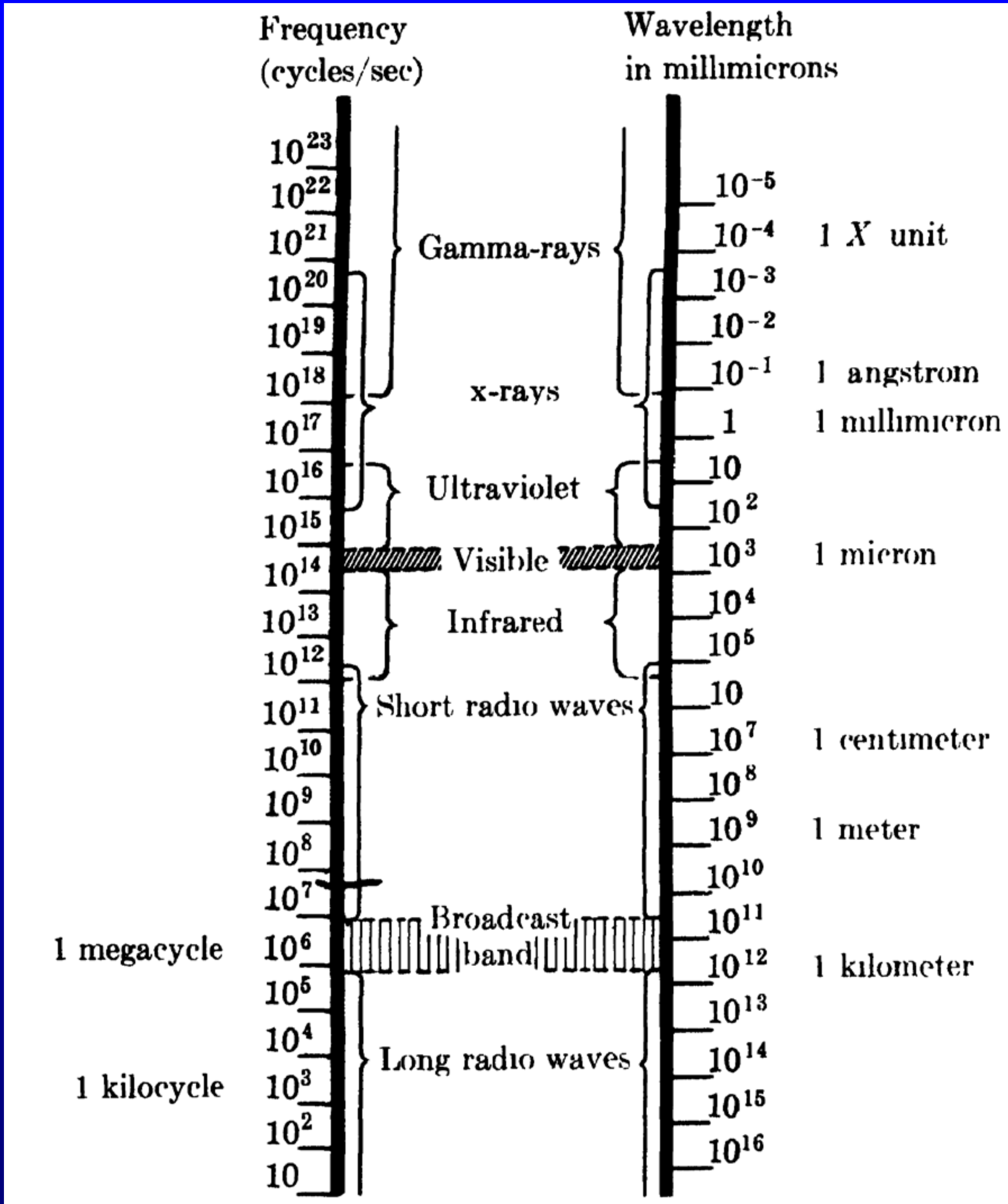
Nature of X-rays

The Discovery of X-Rays

On 8 Nov, 1895, **Wilhelm Conrad Röntgen** (accidentally) discovered an image cast from his cathode ray generator, projected far beyond the possible range of the cathode rays (now known as an electron beam). Further investigation showed that the rays were generated at the point of contact of the cathode ray beam on the interior of the vacuum tube, that they were not deflected by magnetic fields, and they penetrated many kinds of matter.

- A week after his discovery, Rontgen took an X-ray photograph of his wife's hand which clearly revealed her wedding ring and her bones. The photograph electrified the general public and aroused great scientific interest in the new form of radiation. Röntgen named the new form of radiation X-radiation (X standing for "Unknown").



The electromagnetic spectrum.
The boundaries between regions are arbitrary, since no sharp upper or lower limits can be assigned.

1 kX= 1.00202A

Some aspects…

- Invisible
- Penetrating
- Can pass human body, wood, quite thick pieces of metals, and other opaque objects

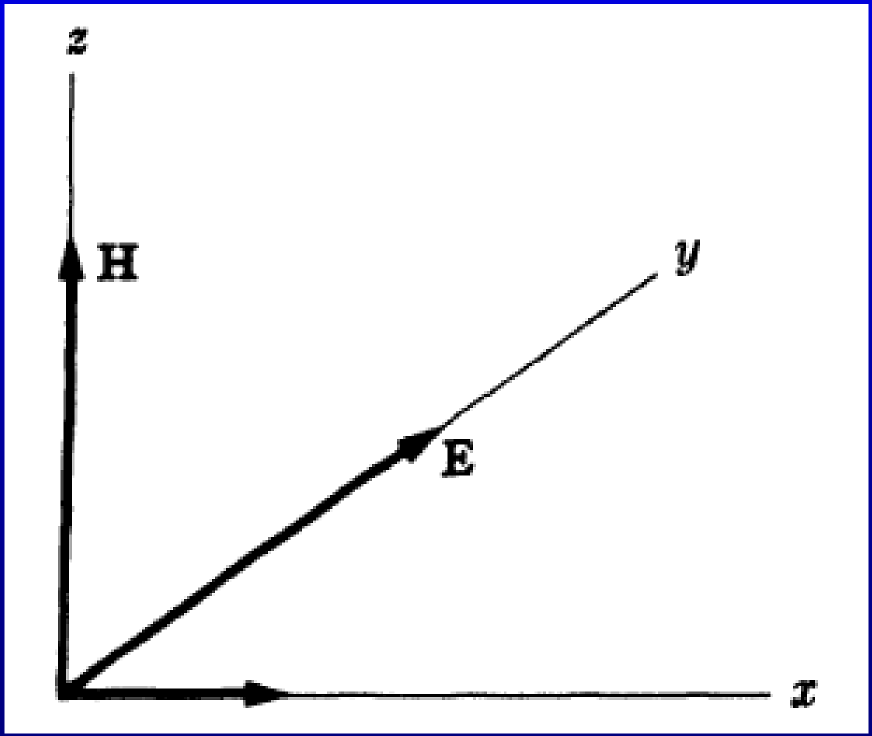
Some aspects…

- Shadow picture-fracture or broken bone-radiography
- Application-started without knowing the properties-till 1912-XRD
- Radiography-resolve 10^{-4} cm = 1 micron
- By diffraction can resolve 10^{-8} cm= 10^{-4} micron = 10^{-1}nm

Electromagnetic radiation

X-rays are electromagnetic radiation and wavelength used for diffraction is in the range of **0.5-2.5 Å**

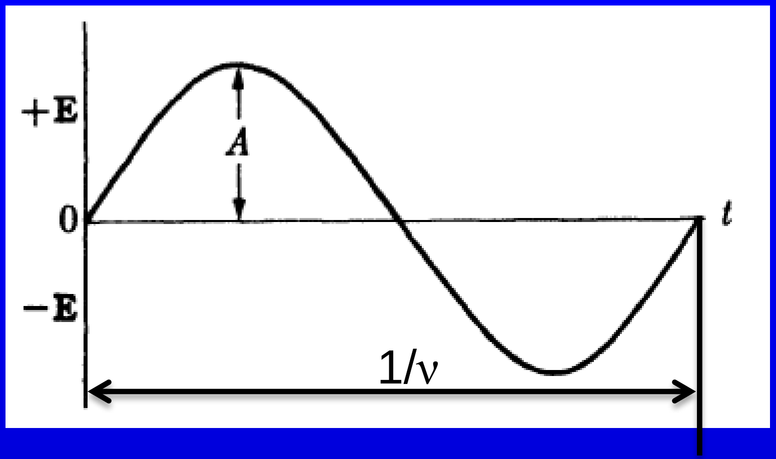
If the electric field is confined to the xy-plane as the wave travels along, the wave is said to be plane polarized.

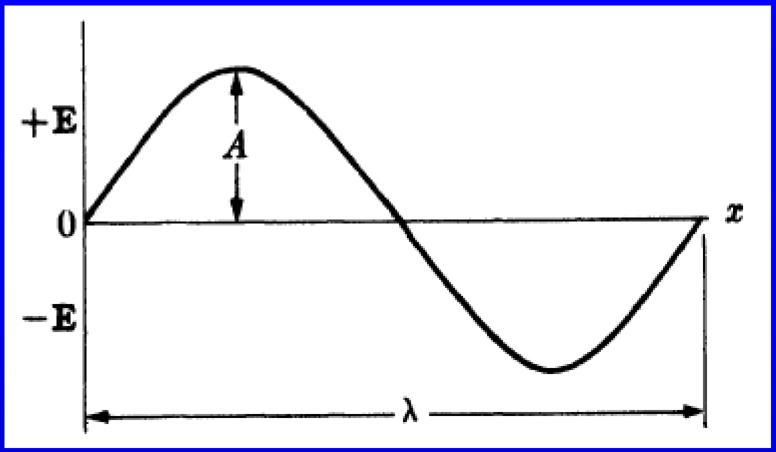


$$\mathbf{E} = A \sin 2\pi \left(\frac{x}{\lambda} - \nu t \right)$$

$$\lambda = \frac{c}{\nu}$$

Electromagnetic radiation





The variation of *E*, (a) with *t* at a fixed value of *x* and (b) with *x* at a fixed value of *t*.

The rate of flow of the energy through unit area perpendicular to the direction of motion of the wave is called the intensity.

Intensity, $I \propto A^2$

Electromagnetic radiation

An accelerated (positive or negative) electric charge radiates energy:

a **charge continuously oscillating** about some mean position acts as an excellent source of electromagnetic radiation.

For example, Radio waves are produced by the oscillation of charge back and forth in the broadcasting antenna

Visible light: oscillating electrons in the atoms of the substance emitting the light.

In each case, **the frequency of the radiation is the same as the frequency of the oscillator which produces it.**

Electromagnetic radiation

Like any other electro-magnetic radiation X-ray has also

Dual nature

Velocity of light = 3.00×10^{8} m/sec

Wave nature $$\lambda = \frac{c}{\nu}$$

Particle nature $$E = h\nu$$

Planck's constant = 6.626×10^{-34} joule.sec

$$E = \frac{ch}{\lambda}$$

Continuous spectrum

In an X-ray tube high velocity of electrons are accelerated toward anode by maintaining high voltage (tens of thousands of volts) across electrodes

High velocity electrons at the point of impact produce X-rays

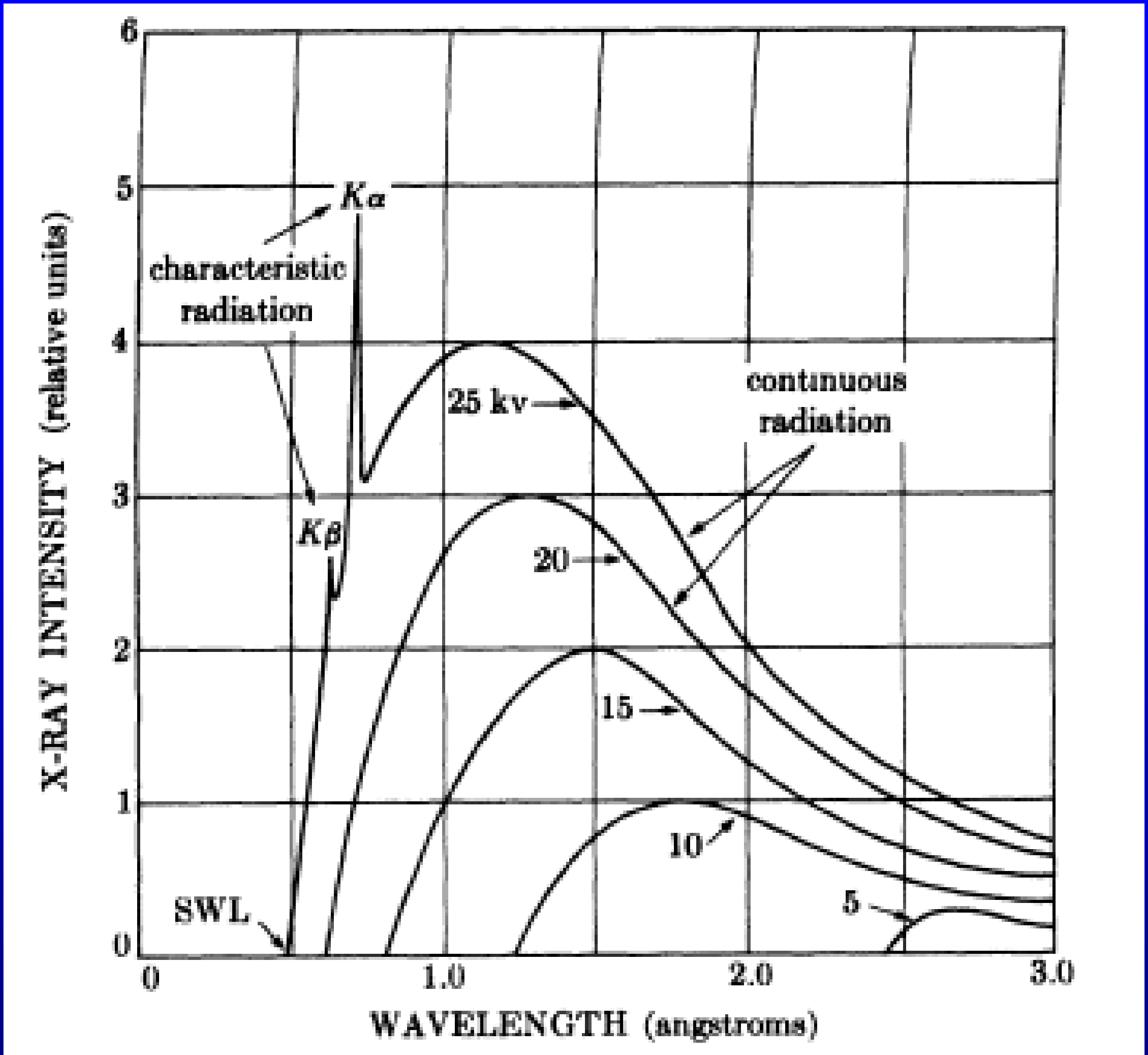
Polychromatic, Continuous spectrum or white radiation (Bremsstrahlung) - X-rays are produced when any electrically charged particle of sufficient kinetic energy is **rapidly decelerated**

Kinetic energy of an electron having charge e (1.6×10^{-19} coulomb) and accelerated by voltage V across the electrodes

$$KE = eV = \frac{1}{2}mv^2$$

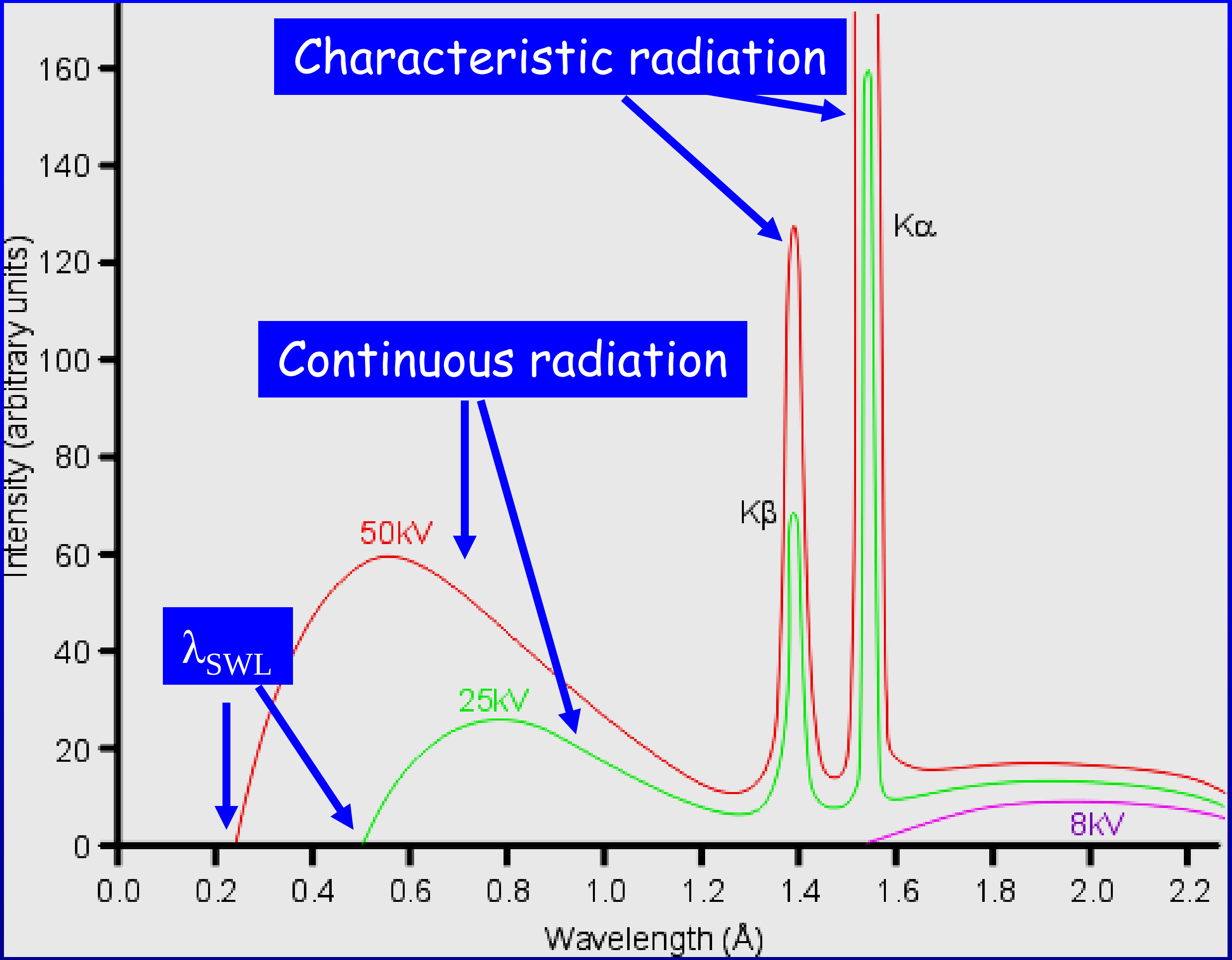
Less than 1 % of the energy of electrons striking the target converts into X-rays

At a tube Voltage of 30,000 V, Velocity of electron is 1/3 of light's velocity!



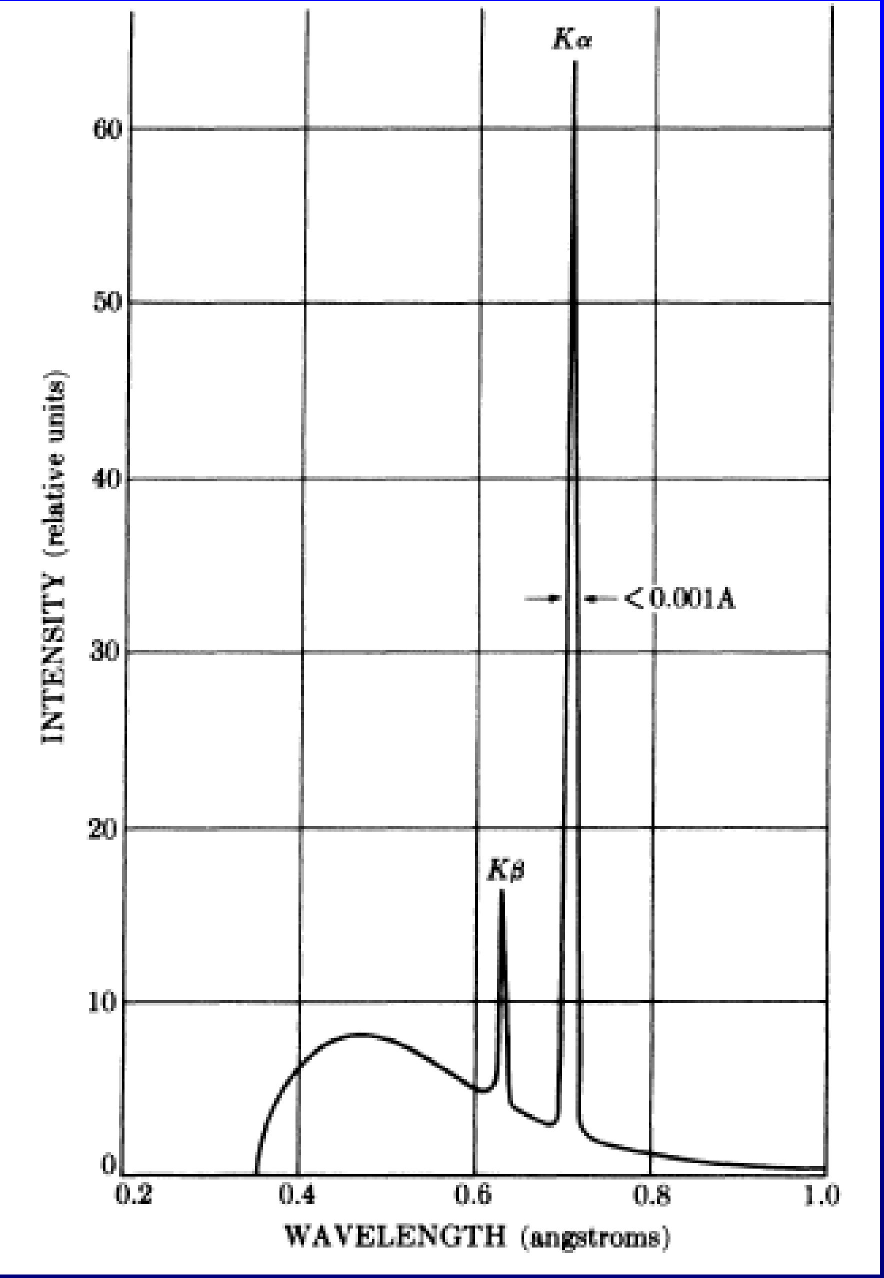
X-ray spectrum of molybdenum as a function of applied voltage (schematic). Line widths not to scale.

Short-wavelength limit (SWL) – Photons of maximum energy, emitted by electrons stopped in one impact



$$\lambda_{SWL} = \lambda_{\min} = \frac{c}{\nu_{\max}} = \frac{hc}{eV}$$

$$\lambda_{SWL} = \frac{12.4 \times 10^3}{V} \text{ Å}$$



Spectrum of Mo at 35 kv (schematic). Line widths not to scale.

X-ray intensities

X-ray intensity of continuous spectrum

$$I_{cont.spect.} = A.i.Z.V^m$$

A is proportionality constant, *m* is a constant with a value of ~2

Intensity of *K* characteristic spectrum

$$I_{\mathrm{K\ line}} = Bi(V - V_K)^n$$

B is proportionality constant, *n* is a constant with a value of ~1.5

Mosley's law - wavelength of any particular line decreased as the atomic number of the emitter increased and he found a linear relationship as:

$$\sqrt{\nu} = C(Z - \sigma)$$

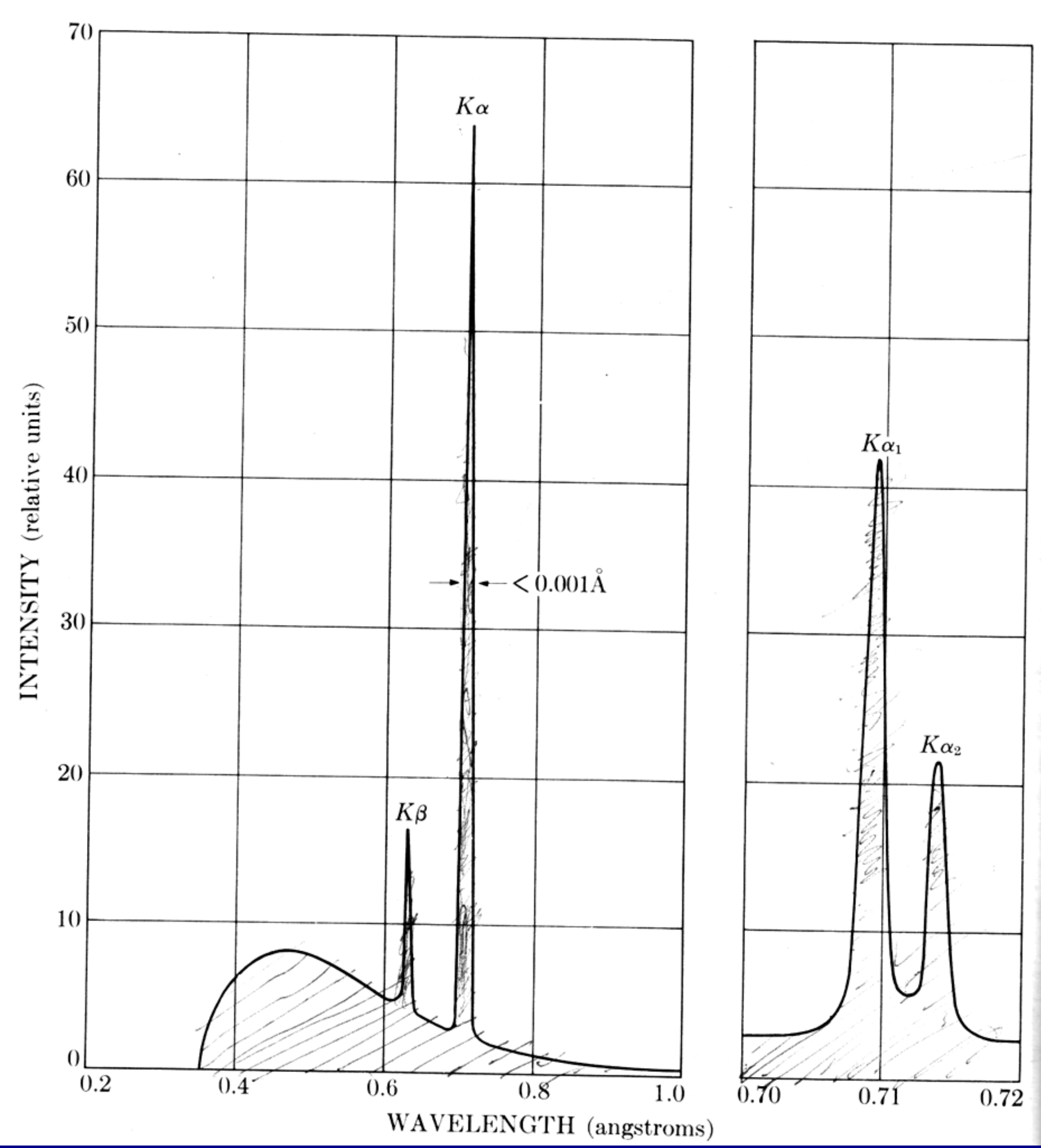
For Molybdenum

$K_{\alpha 1}$ = 0.709 Å

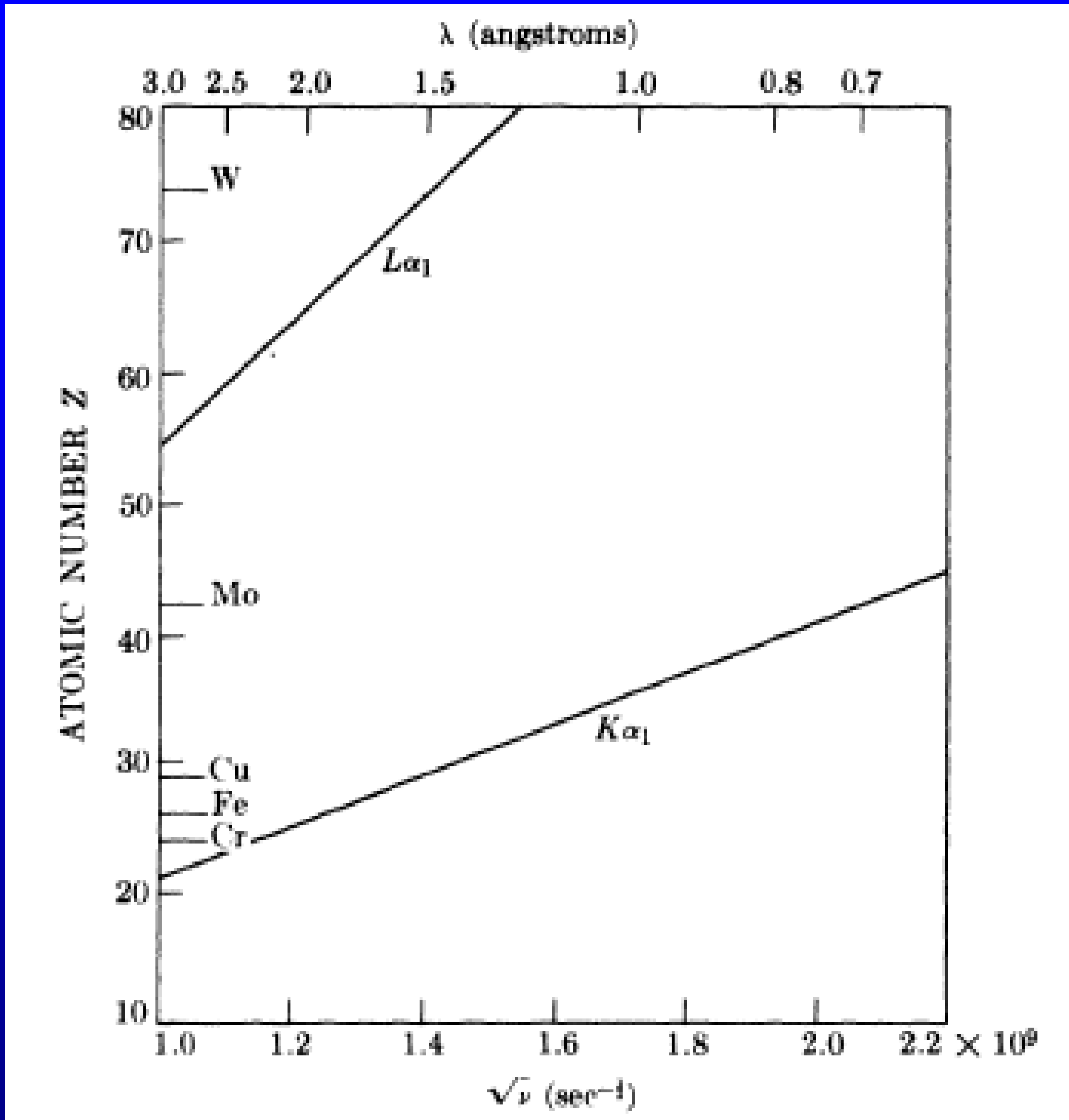
$K_{\alpha 2}$ = 0.714 Å

$K_{\beta 1}$ = 0.632 Å

K_{α} doublet = $\frac{1}{2}(2\times0.709+0.714)$ =0.711 Å



Spectrum of Mo at 35 kV



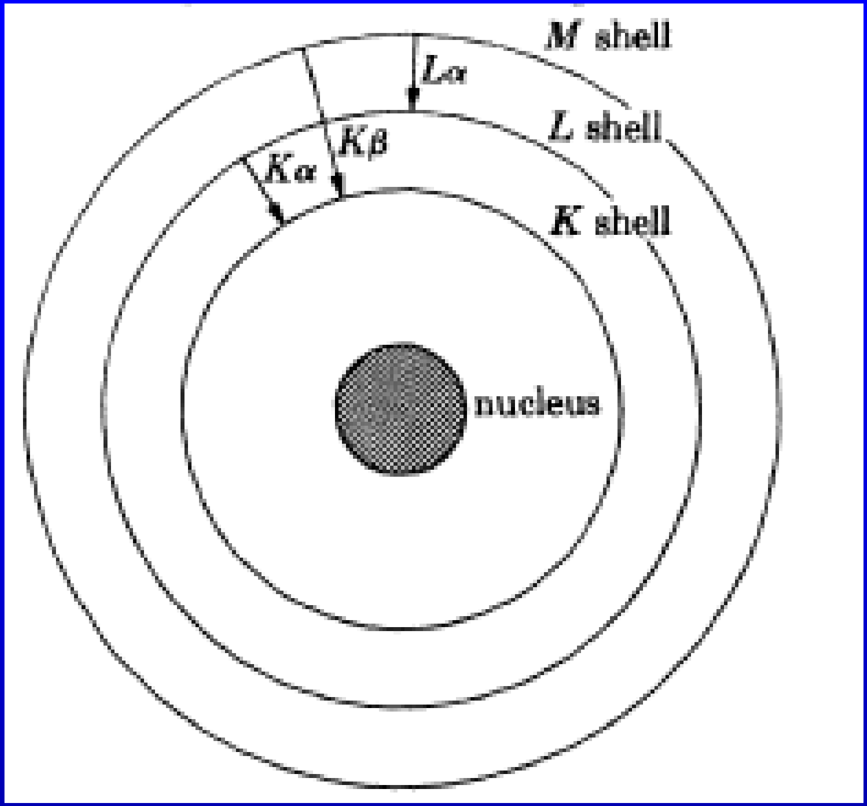
$$\sqrt{\nu} = C(Z - \sigma)$$

This relation is plotted in Fig. for the $K_{\alpha 1}$ and $L_{\alpha 1}$ lines, the latter being the strongest line in the L series.

These curves show, incidentally, that L lines are not always of long wavelength :

the $L_{\alpha 1}$ line of a heavy metal like tungsten, for example, has about the same wavelength as the $K_{\alpha 1}$ line of copper, namely about 1.5A.

Moseley's relation between $\sqrt{\nu}$ and Z for two characteristic lines.



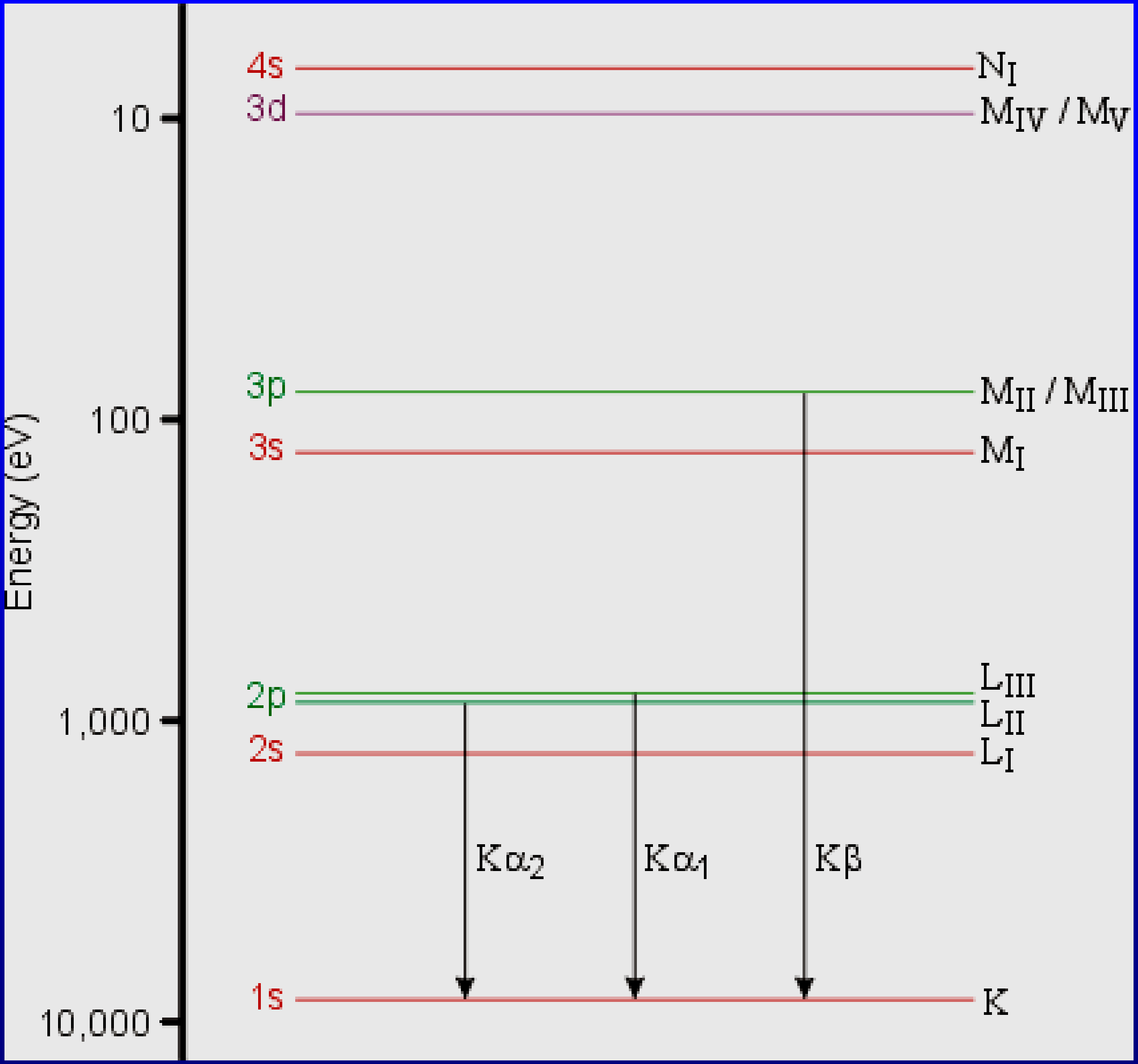
It is impossible to excite one K line without exciting all the others (i.e. L, M etc.).

If W_K is the work required to remove a K electron, then the necessary kinetic energy of the electrons is given by

$$\frac{1}{2}mv^2 = W_k$$

It requires less energy to remove an L electron than a K electron, since the former is farther from the nucleus; it therefore follows that the L excitation voltage is less than the K and that K characteristic radiation cannot be produced without L, M, etc., radiation accompanying it.

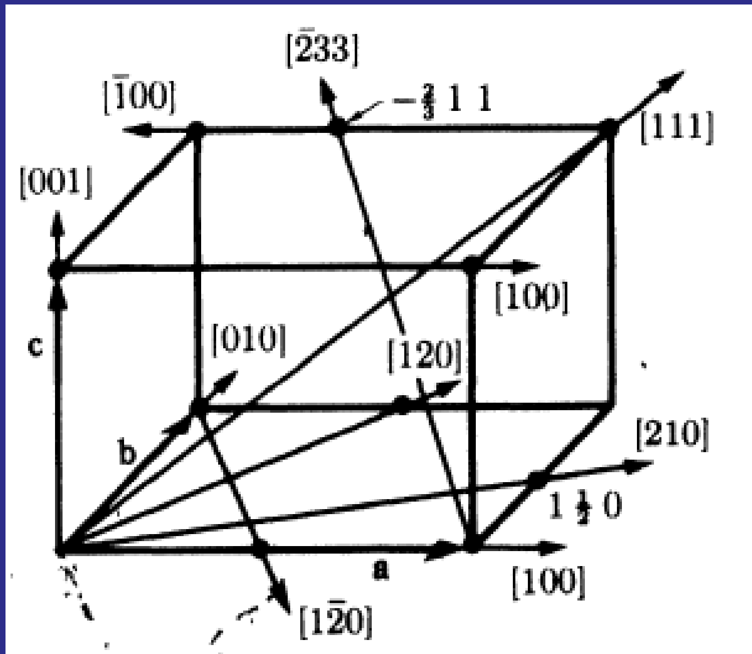
Characteristic radiation

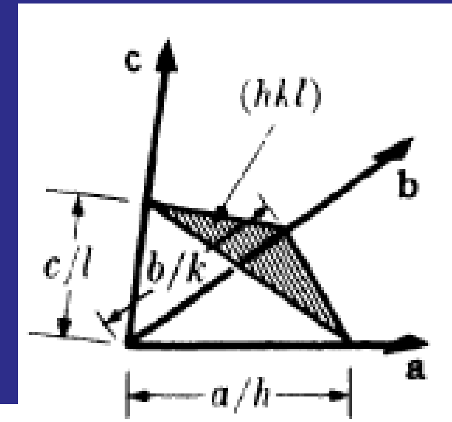


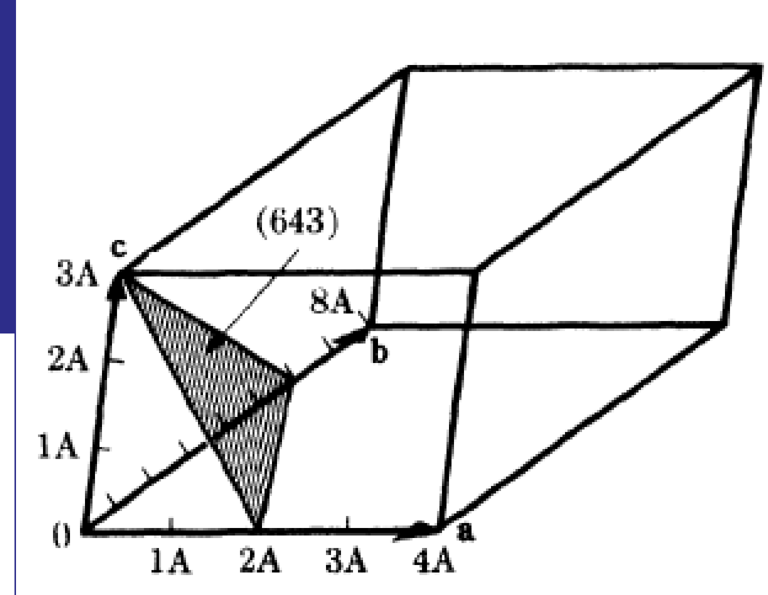
X-Ray Diffraction (XRD)

Few relationships for crystals

Indices for Directions and Planes in Cubic crystals







Axial lengths	4A	8A	3A
Intercept lengths	2A	6A	3A
Fractional intercepts	$\frac{1}{2}$	$\frac{3}{4}$	1
Miller indices	2	$\frac{4}{3}$	1
	6	4	3

Zone axis

Planes of a zone are planes which are all parallel to one line, **called the zone axis,** and the zone, i.e., the set of planes, is specified by giving the indices of the **zone axis**.

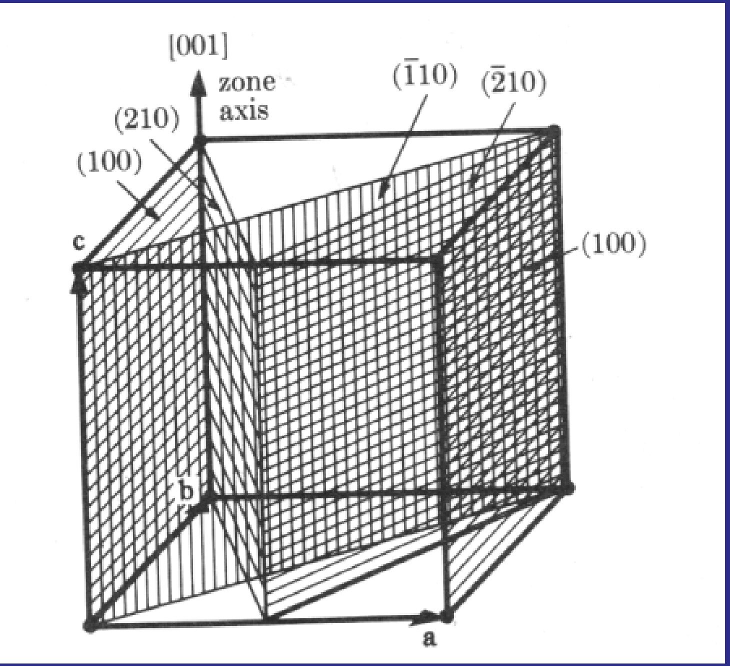
Such planes may have quite different indices and spacings, the only requirement being their parallelism to a line.

$$hu + kv + lw = 0$$

$$u = k_1 l_2 - k_2 l_1$$

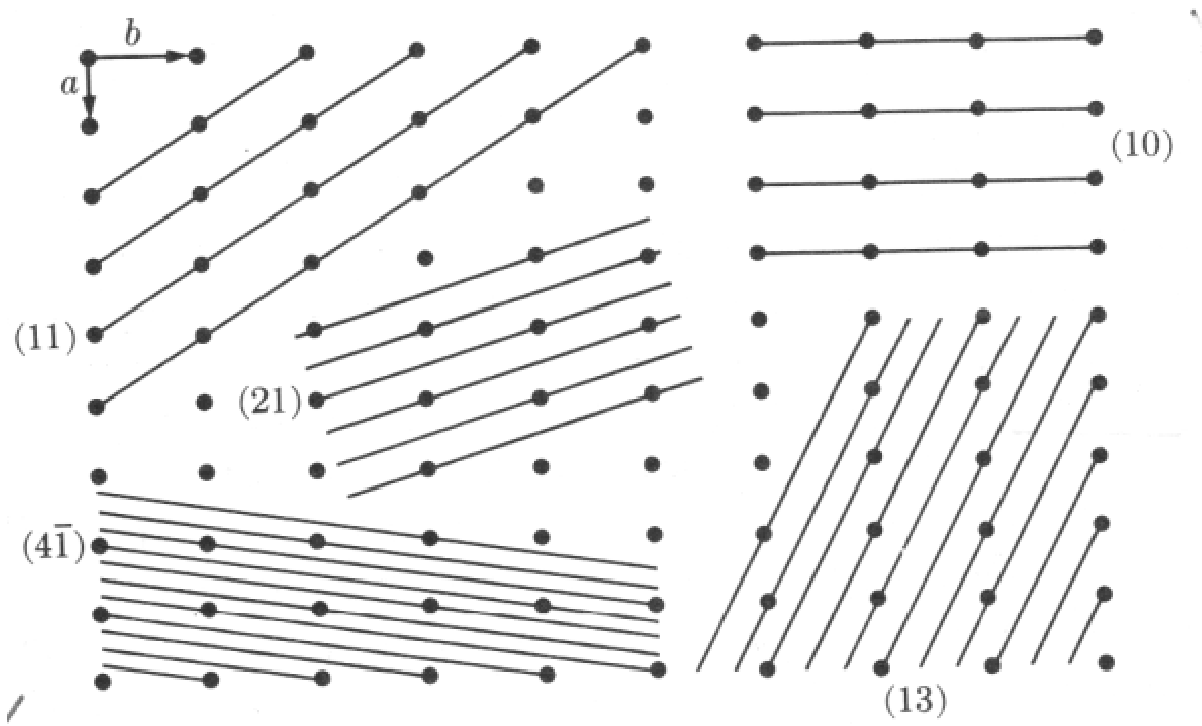
$$v = l_1 h_2 - l_2 h_1$$

$$w = h_1 k_2 - h_2 k_1$$



Lattice spacing

Lines of lowest indices have the greatest spacing and the greatest density of lattice points



Cubic crystal system

$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

Similarity - from prior knowledge

Now you know:

(i) physics of x-rays and (ii) the geometry of crystals

✓phenomenon of x-ray diffraction: Interaction of the above two.

✓Knowledge of crystals: developed by measurement of interfacial angles, chemical analysis, and determination of physical properties.

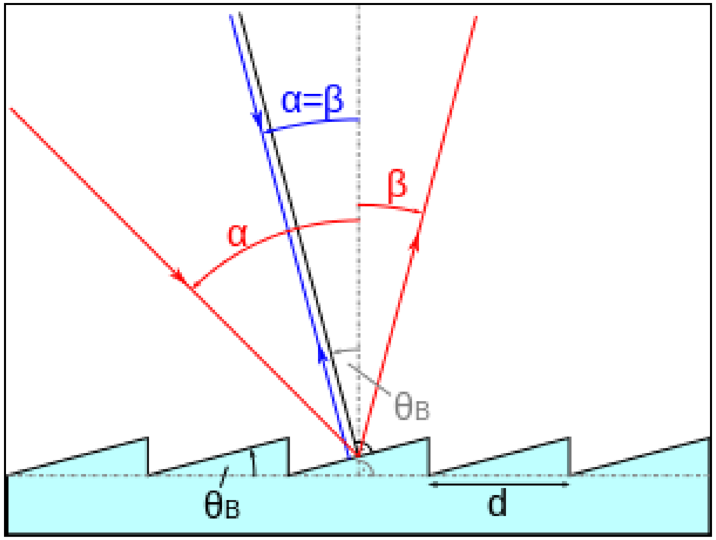
✓Crystal –periodic repetition of atoms/molecules by 1-2 A apart

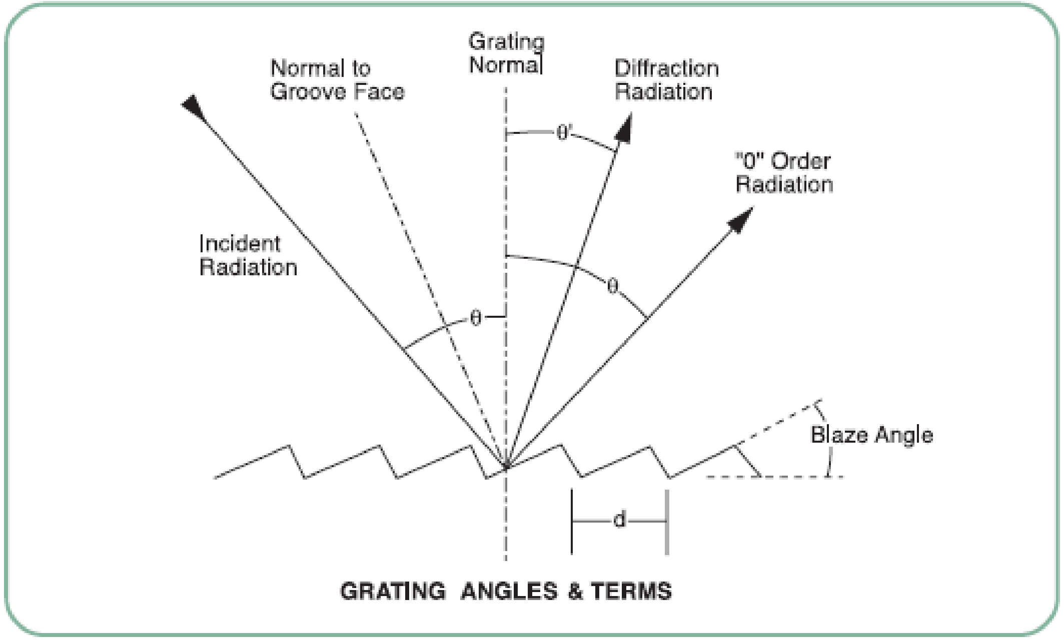
✓X-rays might be electromagnetic wave of wavelength 1-2 A.

▪Diffraction – of visible light by a ruled grating

▪Wave encounter set of regularly spaced scattering objects

▪Wavelength of wave in question has same order of magnitude as of spacing between scattering centers.





German physicist von Laue reasoned

He reasoned that if crystals are composed of regularly spaced atoms - can act as scattering centers for x-rays

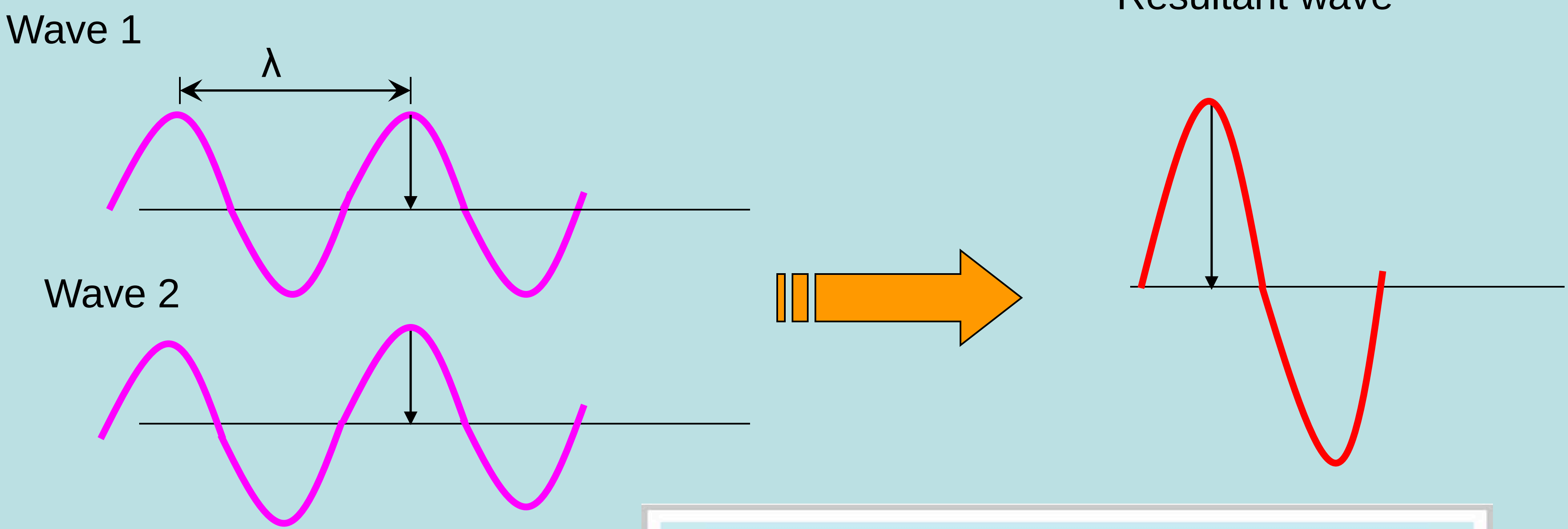
If x-rays have wavelength about equal to inter-atomic distance in crystal, it should be possible to diffract x-rays by means of crystals

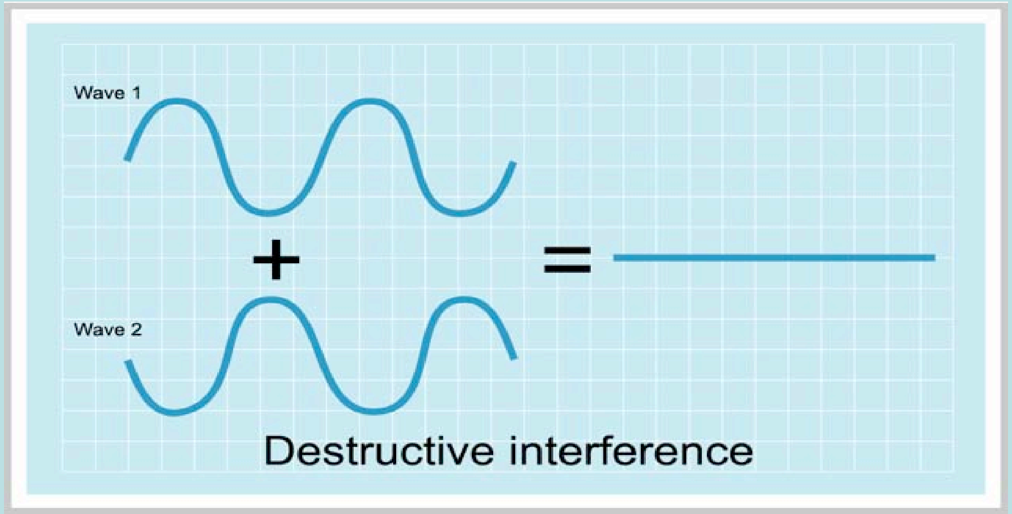
Copper sulphate test proves:

1. the wave nature of x-rays and

2. the periodicity of the arrangement of atoms within a crystal.

Constructive – Destructive Interference

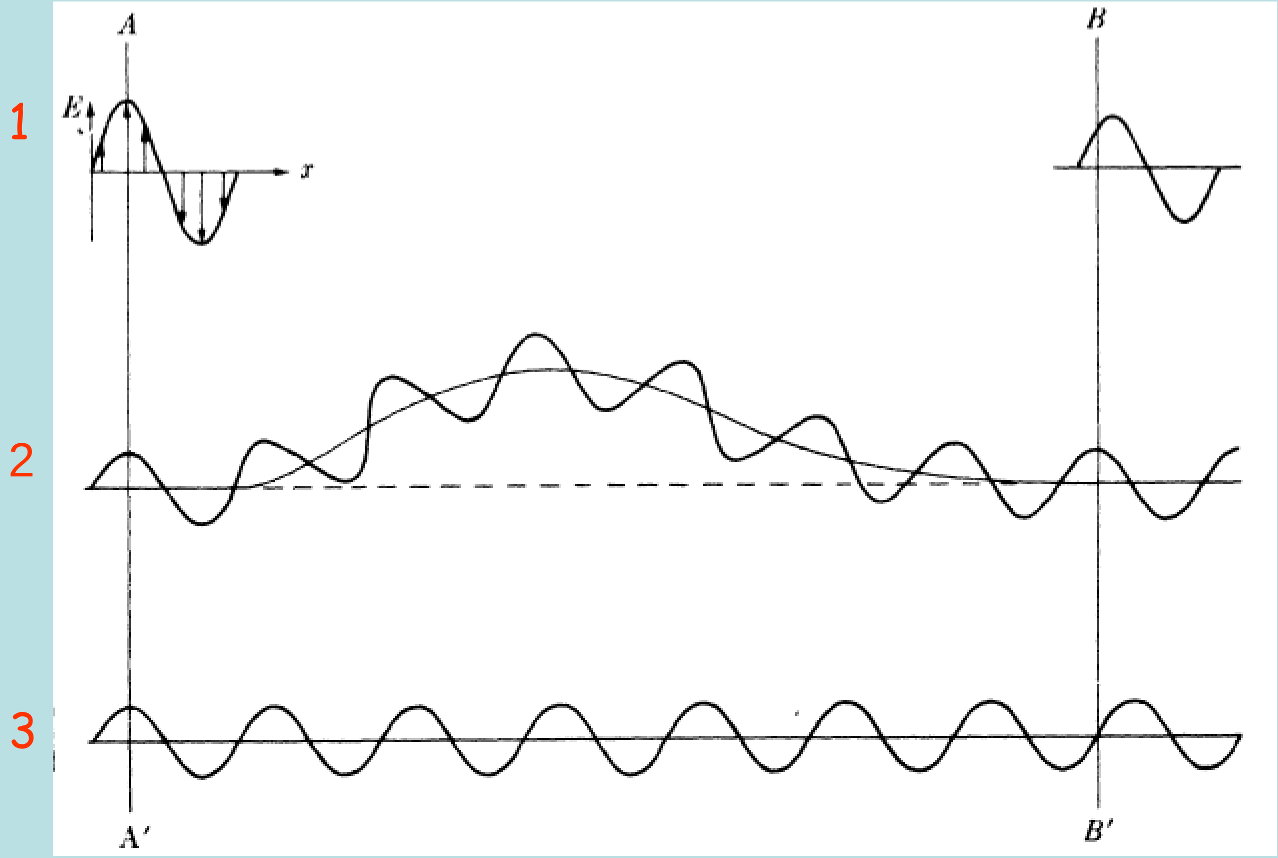




Differences in the length of the path traveled lead to differences in phase

The introduction of phase differences produces a change in amplitude

Diffraction is due to the existence of phase relationship between 2 or more waves.



Effect of path difference on relative phase.

Two conclusions may be drawn from this illustration :

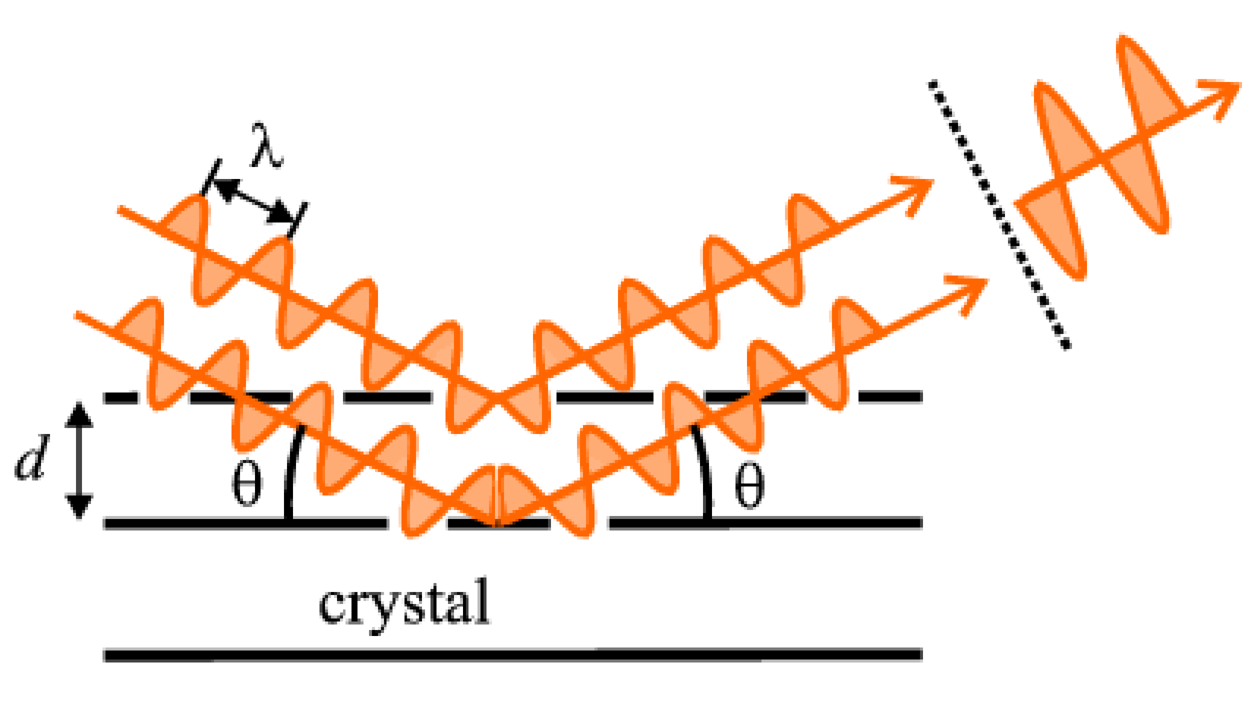
(1) Differences in the length of the path traveled lead to differences in phase.

(2) The introduction of phase differences produces a change in amplitude.

The greater the path difference, the greater the difference in phase,

Since the path difference measured in wavelengths, exactly equals the phase difference, also measured in wavelengths.

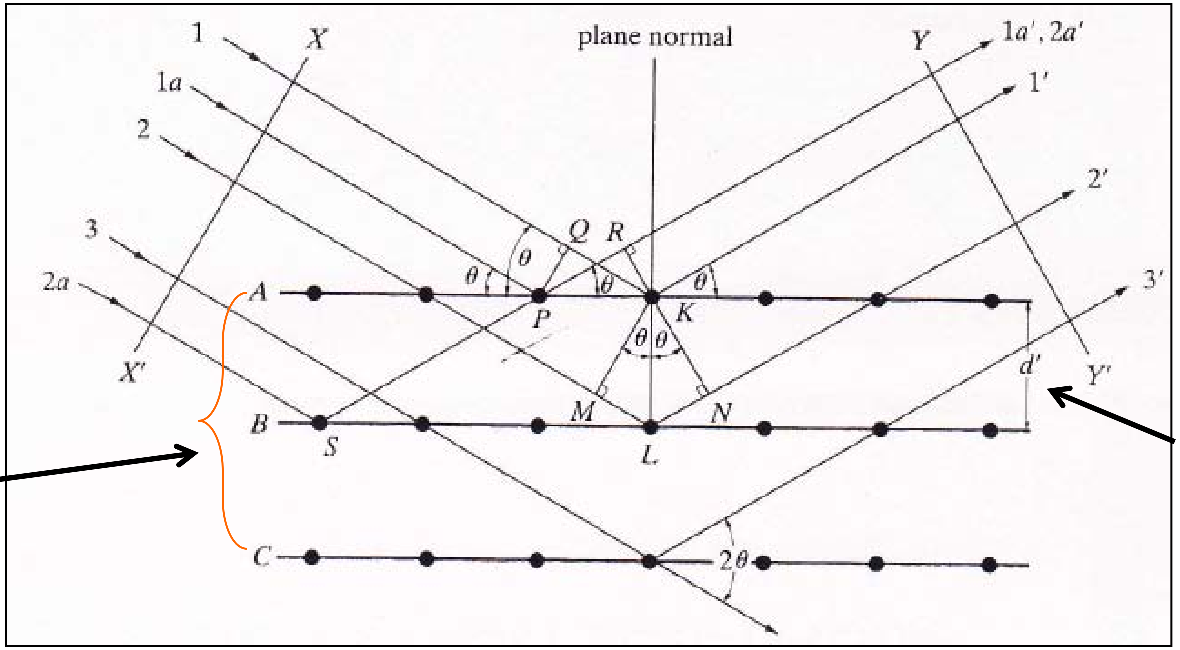
two rays are completely in phase whenever their path lengths differ either by zero or by whole number of wavelengths.



A diffracted beam may be defined as a beam composed of a large number of scattered rays mutually reinforcing one another.

Diffraction

Simplification given W. H. Bragg and W. L. Bragg



Crystal planes- imaginary

interplanar spacing

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

Essential condition for diffraction

The difference in the length of path between the diffracted rays,**1 &1a'** and wave fronts XX' and YY' is equal to

$$QK - PR = PK\cos\theta - PK\cos\theta = 0.$$

Rays 1 and 2 are scattered by atoms K and L, and the path difference for rays 1K1' and 2L2' is

$$ML + LN = d'\sin\theta + d'\sin\theta.$$

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

- The **diffracted beam is stronger** compared to the sum of all the rays scattered in the same direction, simply because of the **reinforcement** which occurs,

- But, it is extremely **weak compared to the incident beam** since the atoms of a crystal **scatter only a small fraction of the energy** incident on them.