X-ray Diffraction

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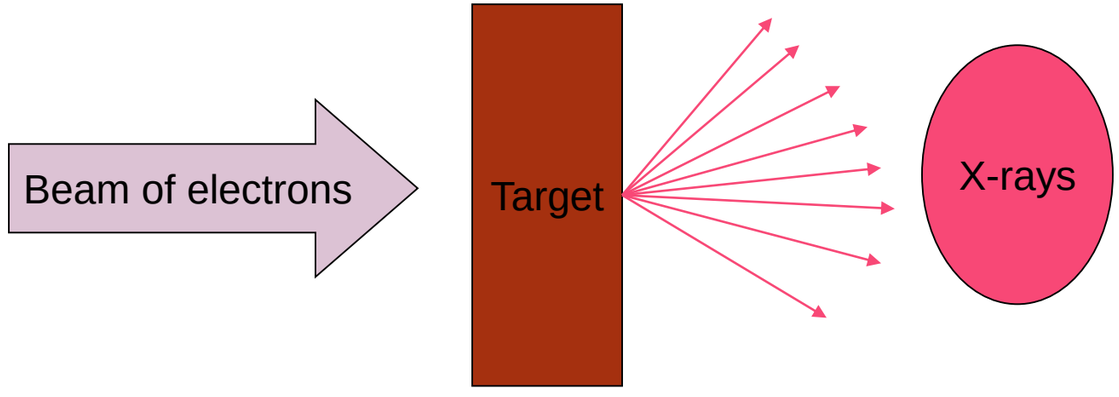
X-ray diffraction

Why diffraction is used to find out crystal structure?

- Atoms are periodically arranged and acts as a 3-D grating.
- The interatomic spacing is around 2-3 Å, so a ray should have wavelength matching to grating.
- X-rays are having identical wavelength to atomic spacing.

Generation of X-rays

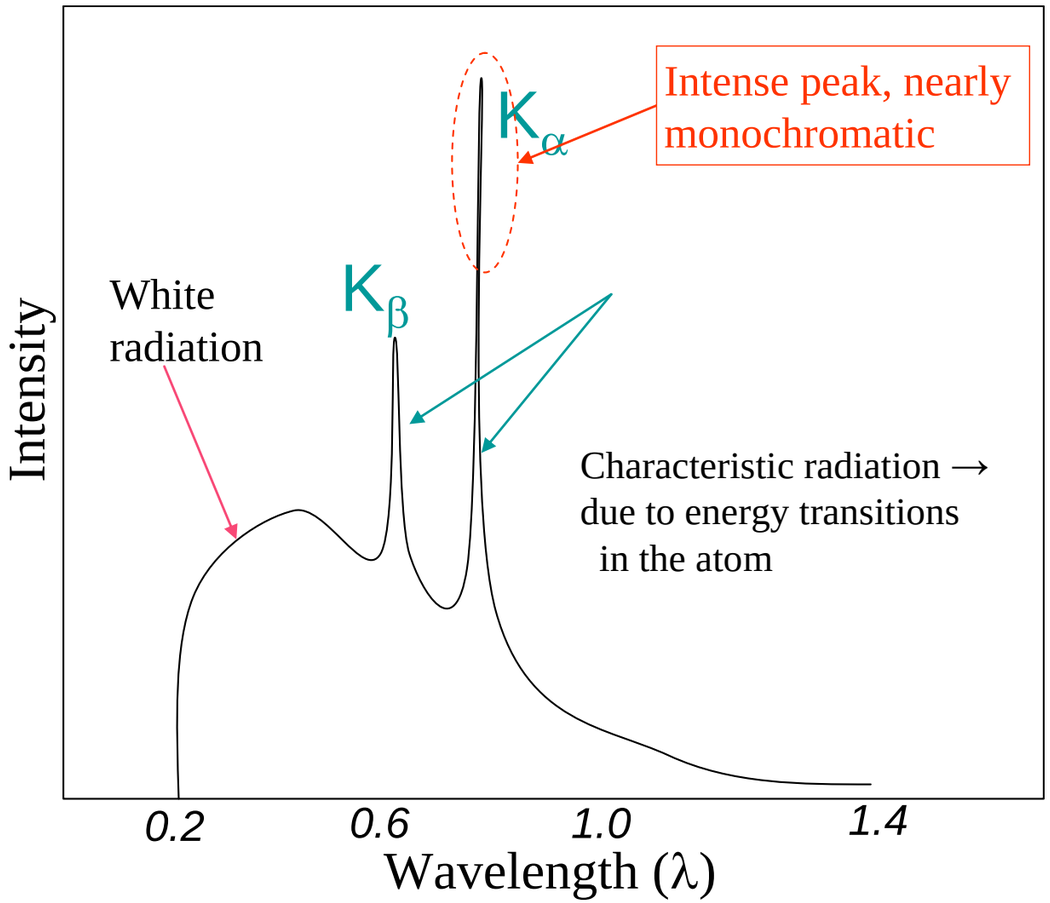
- X-rays can be generated by decelerating electrons.
- Hence, X-rays are generated by bombarding a target (say Cu) with an electron beam.

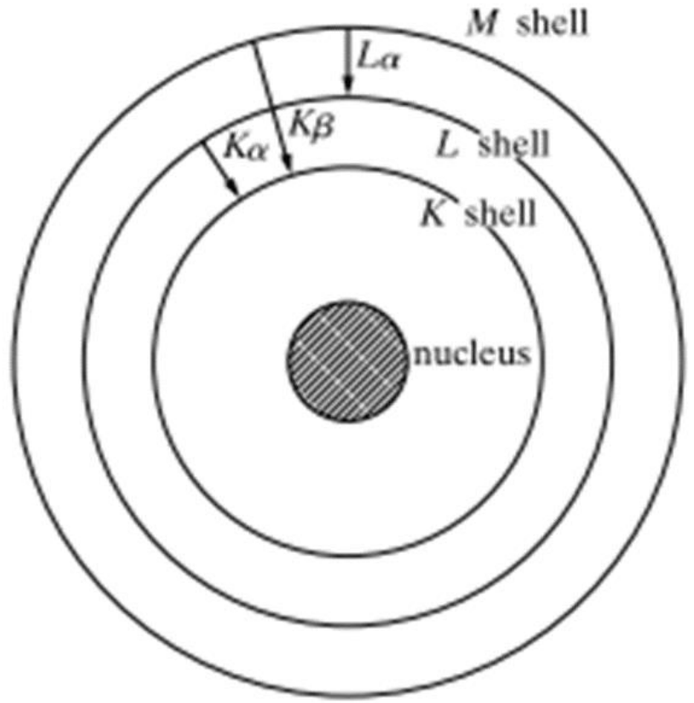


An accelerating (or decelerating) charge radiates electromagnetic radiation

Generation of X-rays

- The resultant spectrum of X-rays generated (i.e. $\lambda_{X\text{-rays}}$ versus Intensity plot) shows intense peaks on a 'broad' background.
- The intense peaks can be 'thought of' as monochromatic radiation and be used for X-ray diffraction studies.



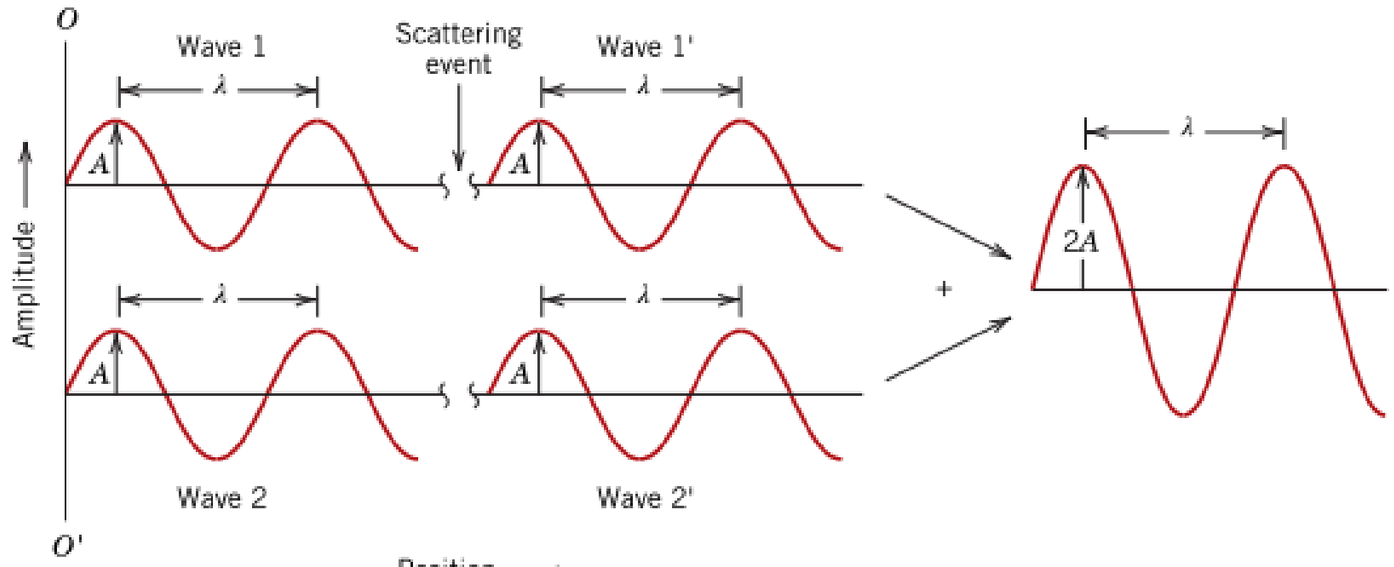


Can every metal generate X-rays?

Yes, with exception, most of the metals.

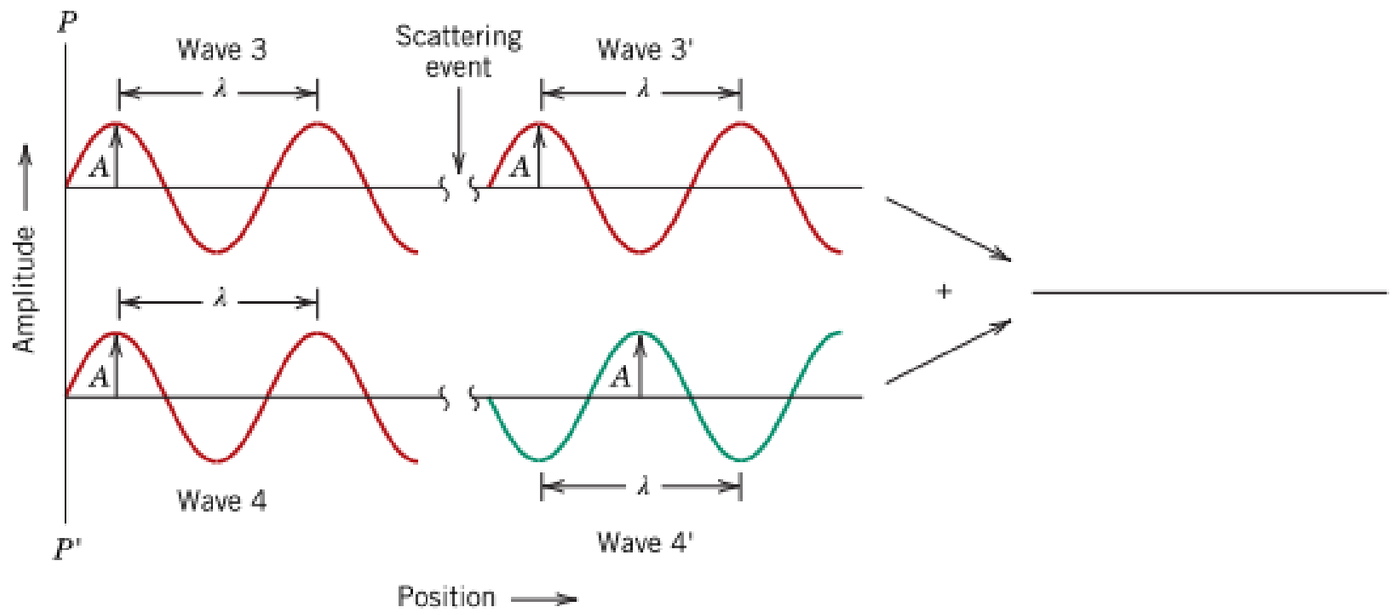
Elements	(KV)	λ Of $K_{\alpha 1}$ radiation (Å)	λ Of $K_{\alpha 2}$ radiation (Å)	λ Of K_{β} radiation (Å)
Ag	25.52	0.55941	0.5638	0.49707
Mo	20	0.7093	0.71359	0.63229
Cu	8.98	1.540598	1.54439	1.39222
Ni	8.33	1.65791	1.66175	1.50014
Co	7.71	1.78897	1.79285	1.62079
Fe	7.11	1.93604	1.93998	1.75661
Cr	5.99	2.2897	2.29361	2.08487

The diffraction phenomenon



(a)

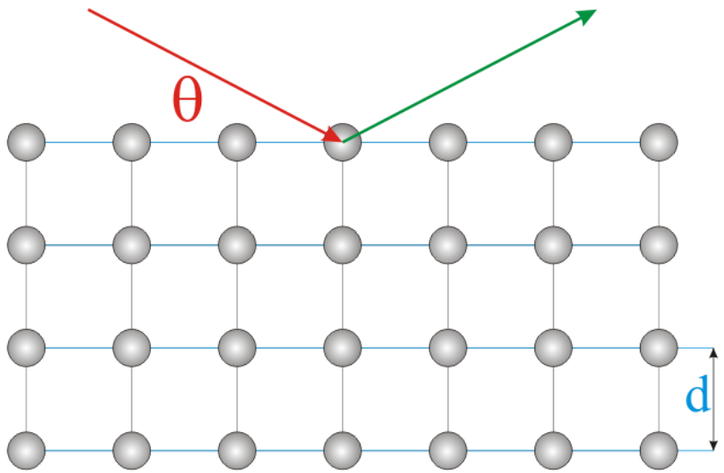
Constructive Interference

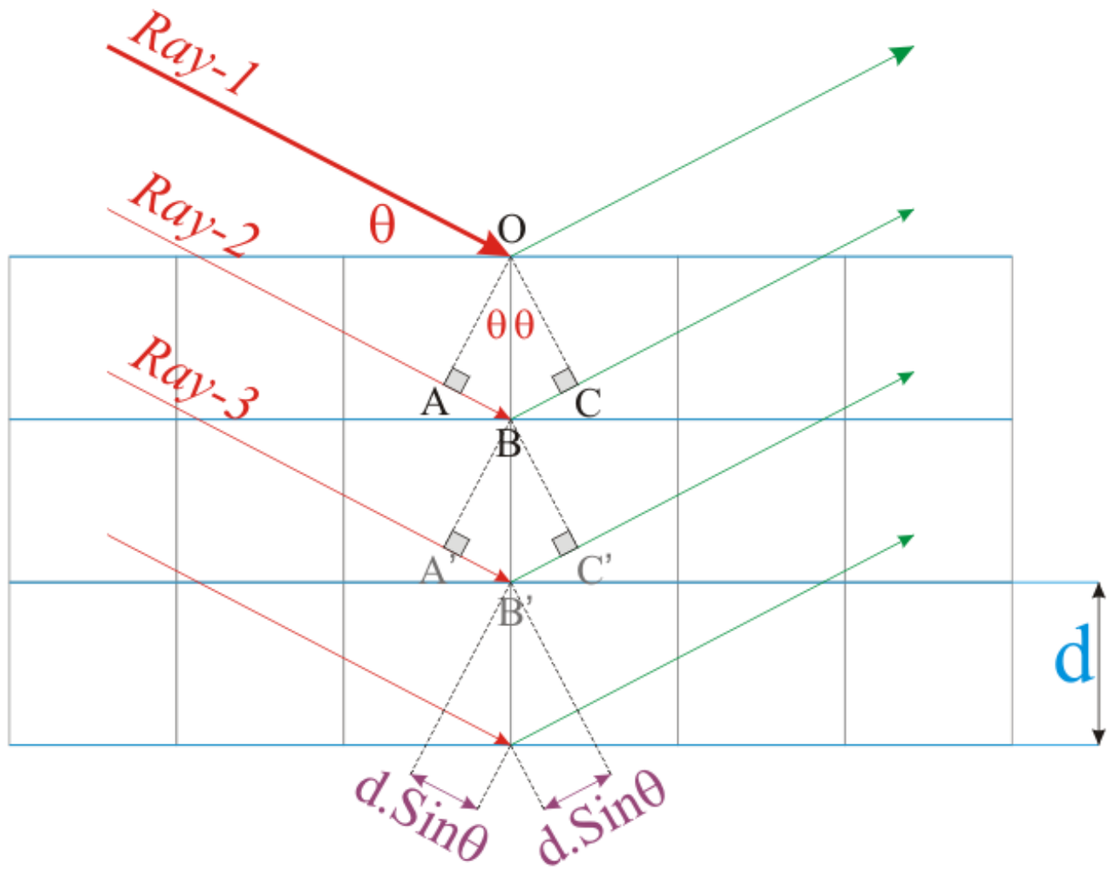


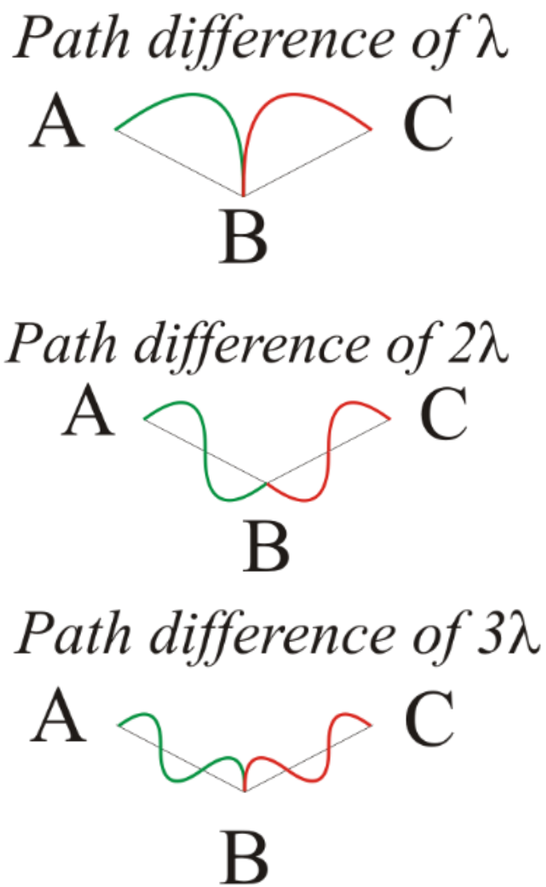
Destructive Interference

The Bragg's law

Let us consider scattering across planes





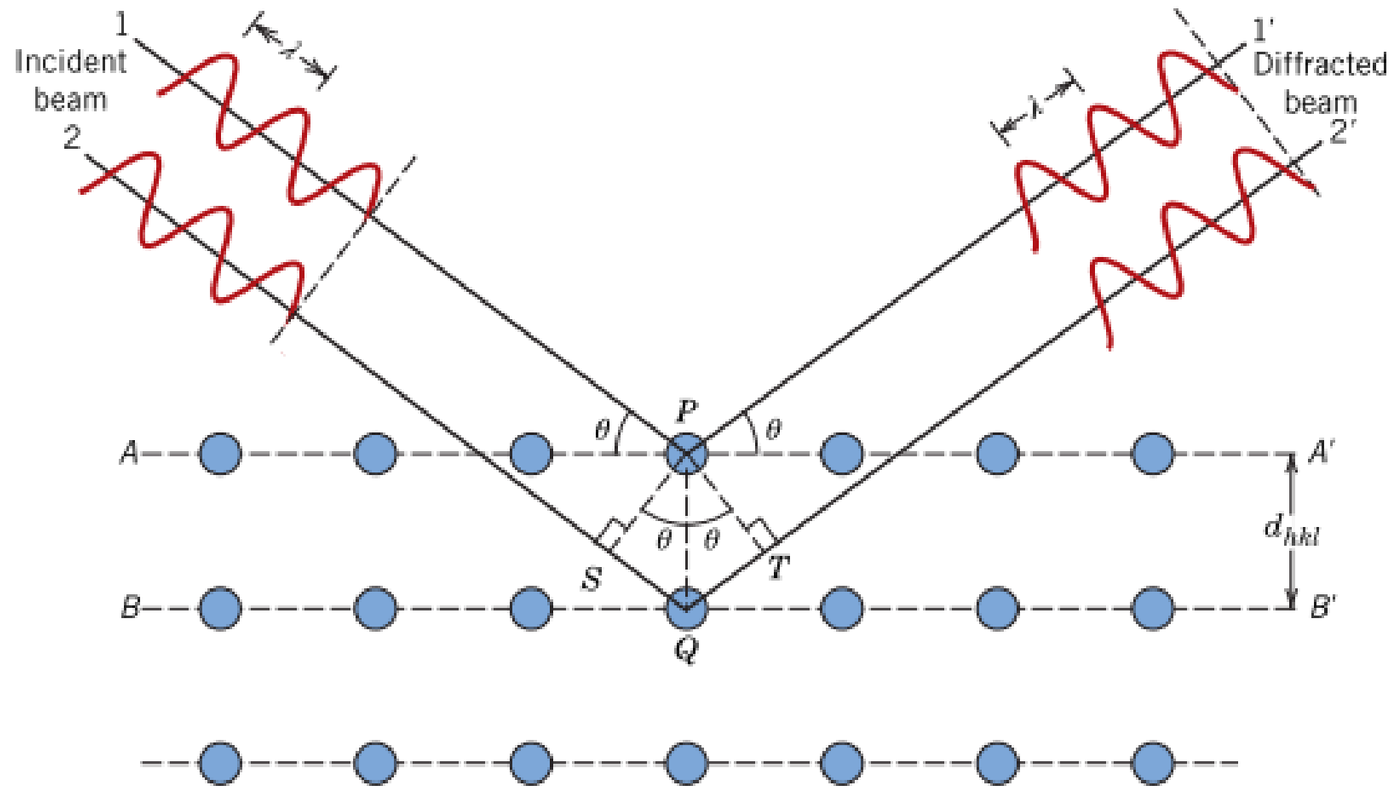


Ray-1, ray-2 and ray-3 are constructively interfering. As the path difference is in multiple of λ.

So intensities will add up.

The Bragg's Law

$2d\sin\theta = n\lambda$ ➔ Bragg's equation



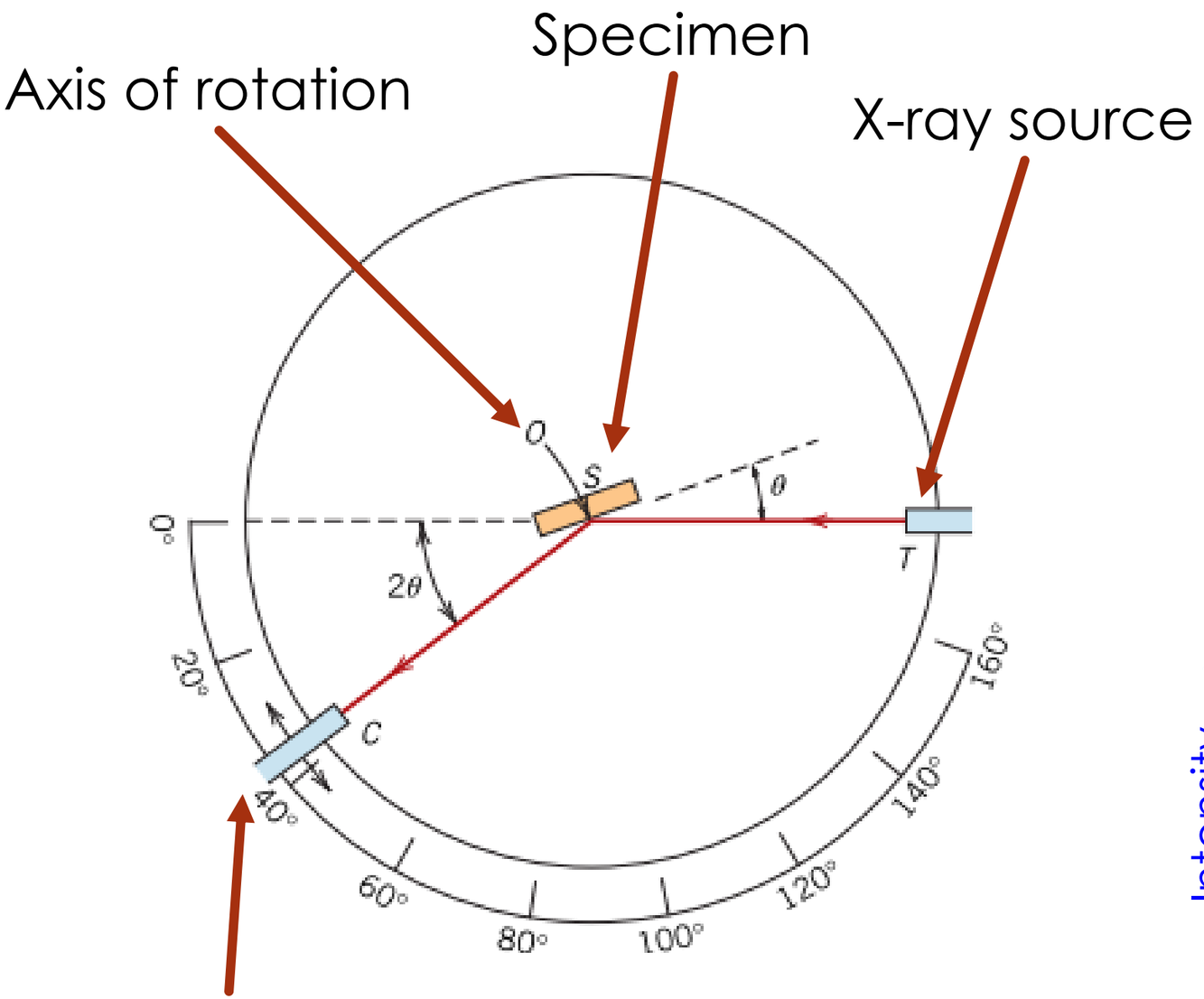
If Bragg's eq. is NOT satisfied → NO 'reflection' can occur
If Bragg's eq. is satisfied → 'reflection' *MAY* occur

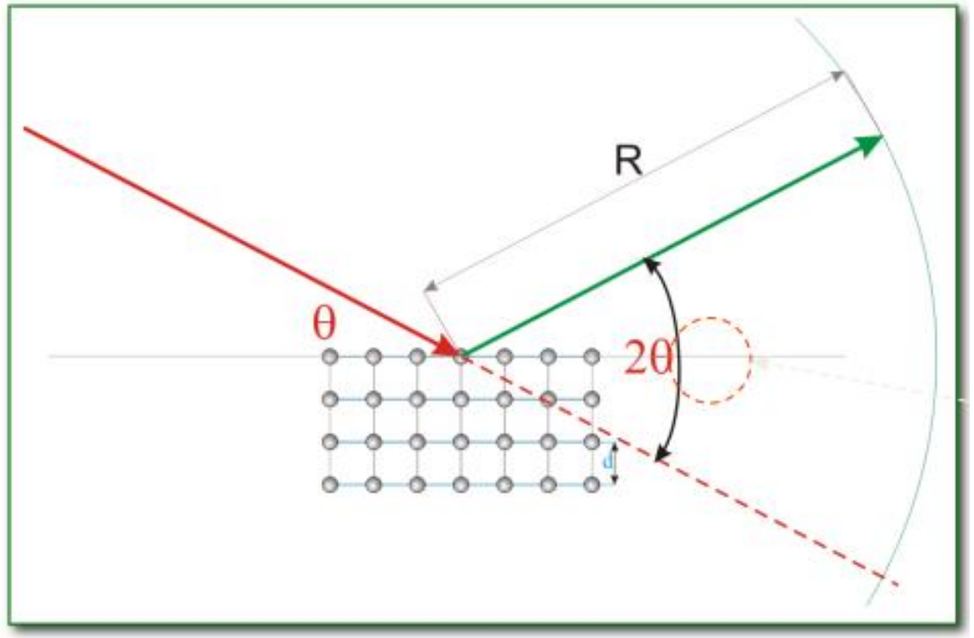
Remember

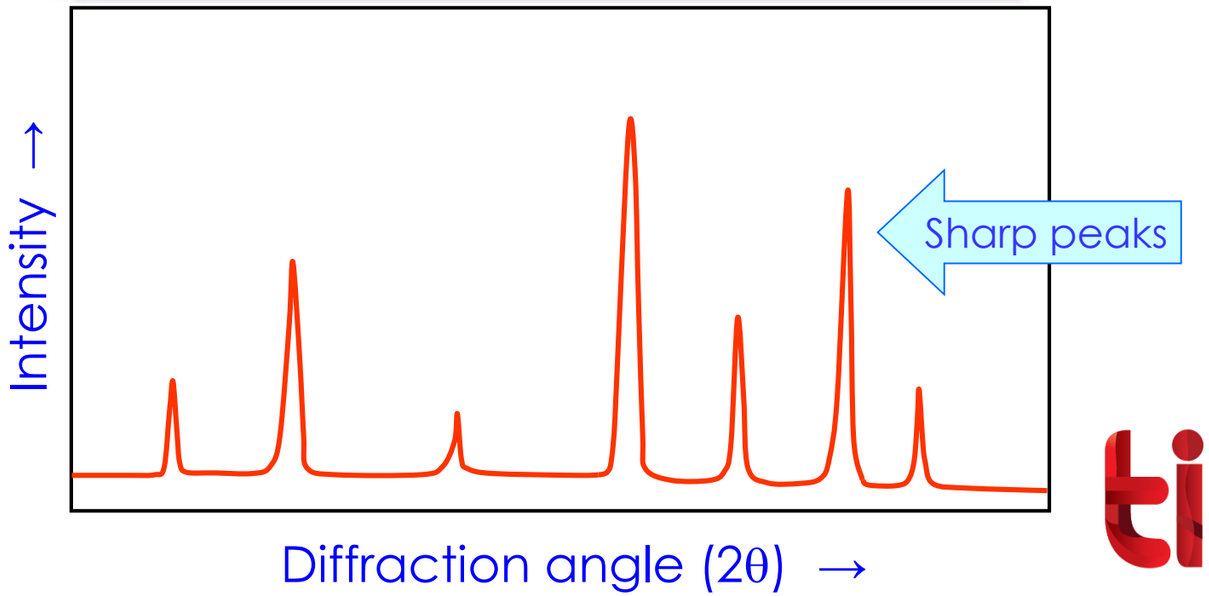
- X-rays have matching wavelength to the interplanar spacing (2 – 3 Å).
- If there is a constructive interference, then diffraction occurs.
- For diffraction, X-ray should be monochromatic, having high intensity and matching wavelength to the lattice spacing.

X-ray powder diffraction method

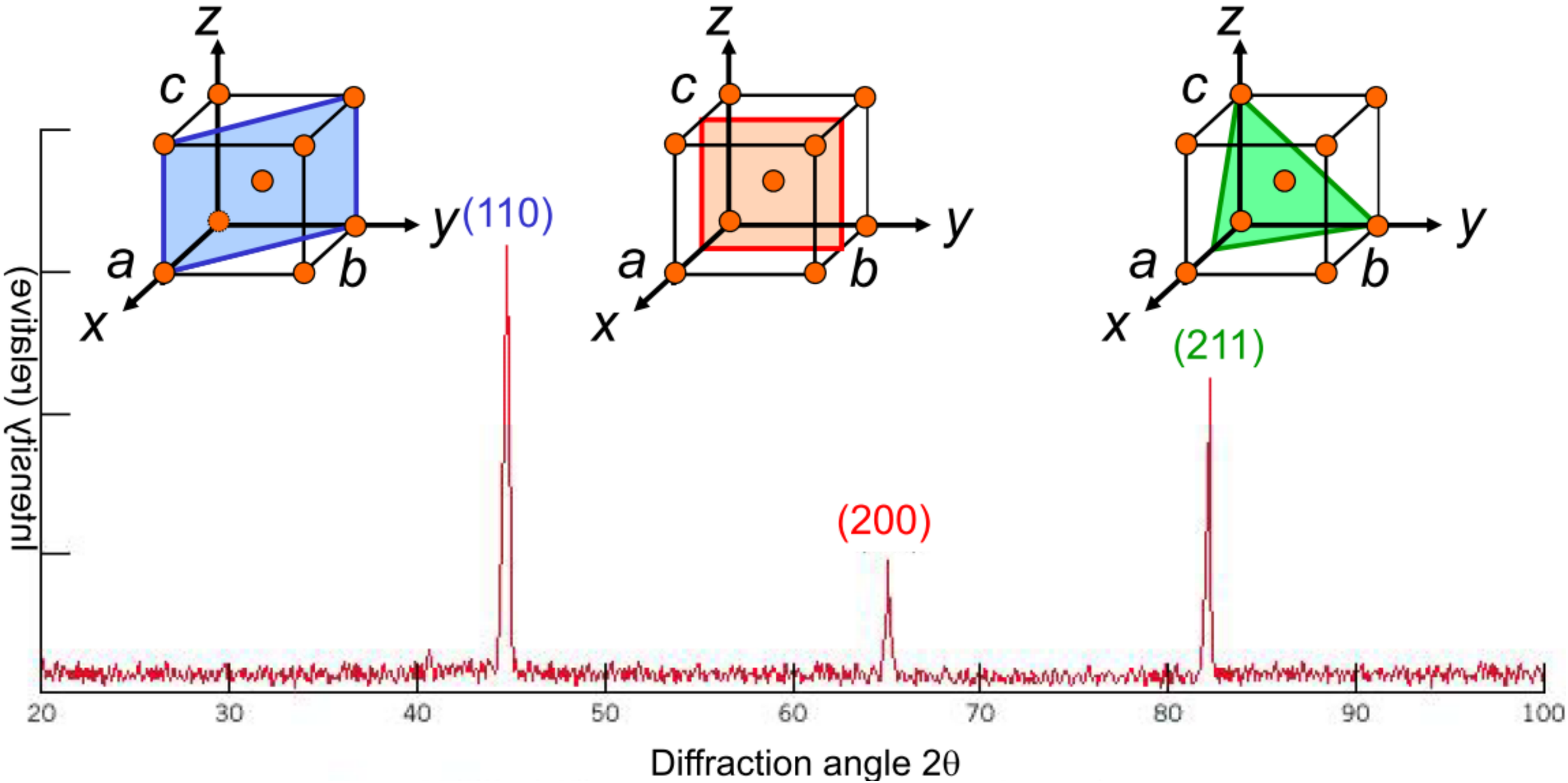
How the diffraction measurement takes place?







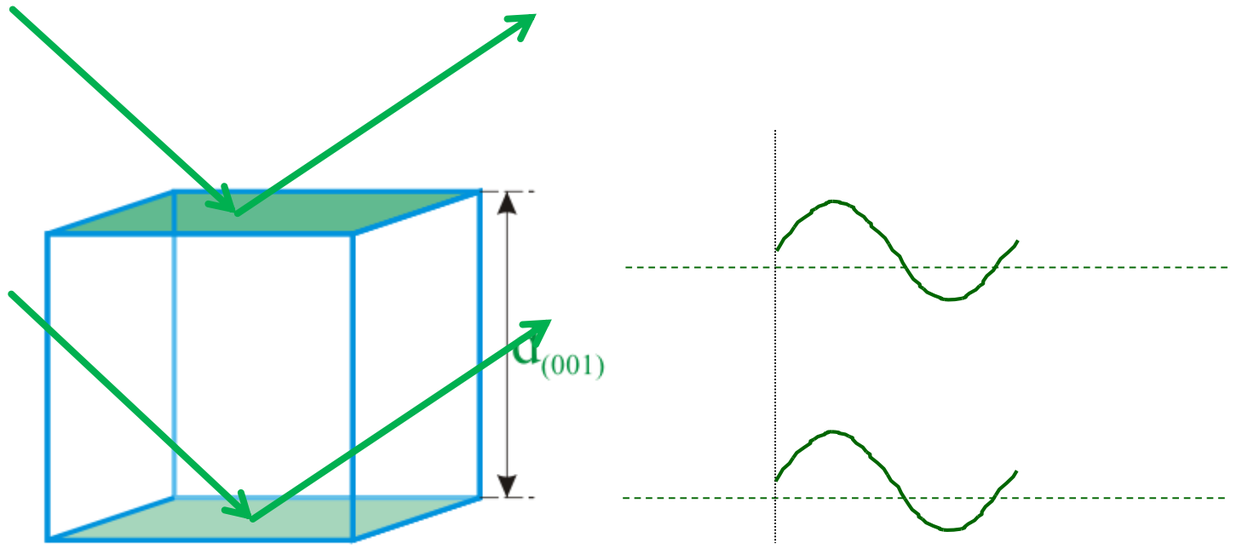
X-ray powder diffraction pattern



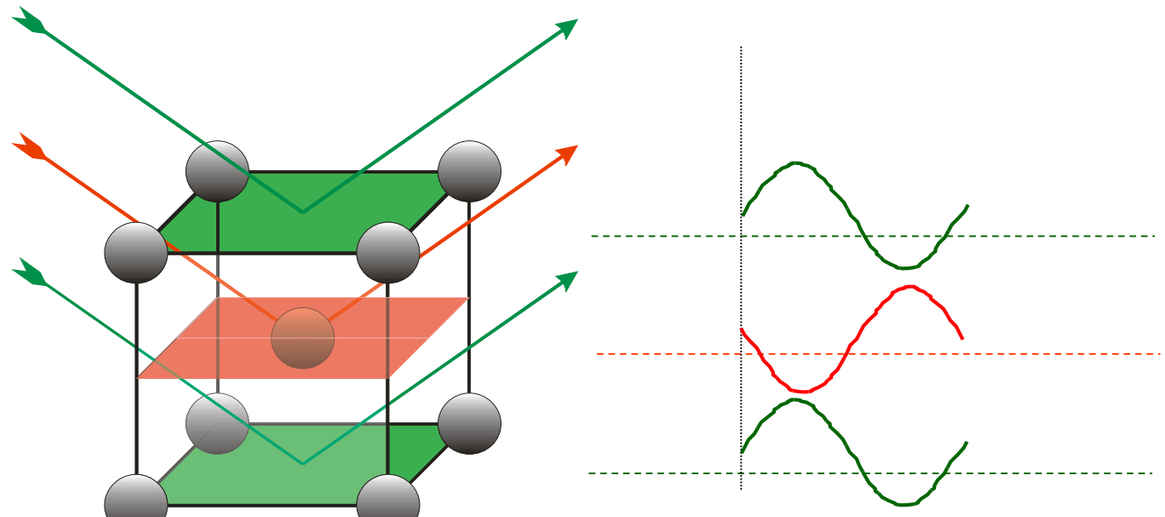
X-ray powder diffraction

Does every plane give reflection/signal

Simple cubic



Body centered cubic



The diffraction from (100) planes get cancelled out by the extra atom at the center in BCC.

So (100) reflection is absent in BCC.

Summary

1. For diffraction, X-ray should be monochromatic, having high intensity and matching wavelength to the lattice spacing.
2. X-rays have matching wavelength to the interplanar spacing (2 – 3 Å).
3. If there is a constructive interference, then and only then diffraction occurs.