First QUIZ of MLL100

Date	: *January 25, 2022*
Day	: *Tuesday*
Time	: *10:30 a.m. – 10:50 a.m.*
Marks	: *10*
Mode	: *Online (Moodle)*
Syllabus	: *Topics covered until Jan 19, 2022*

MLL 100

Introduction to Materials Science and Engineering

Lecture-7 (January 18, 2022)

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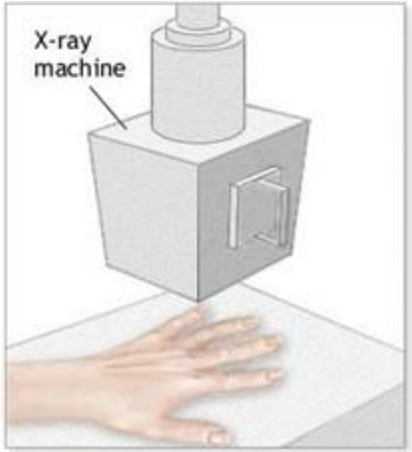
Department of Materials Science and Engineering

Topics covered

- Miller-Bravais indices of planes and directions in a hexagonal system


HAVE YOU SUFFERED A BROKEN BONE
IN A SLIP AND FALL?
Hupy and
Abraham s.c.
hupy.com

X-ray diffraction



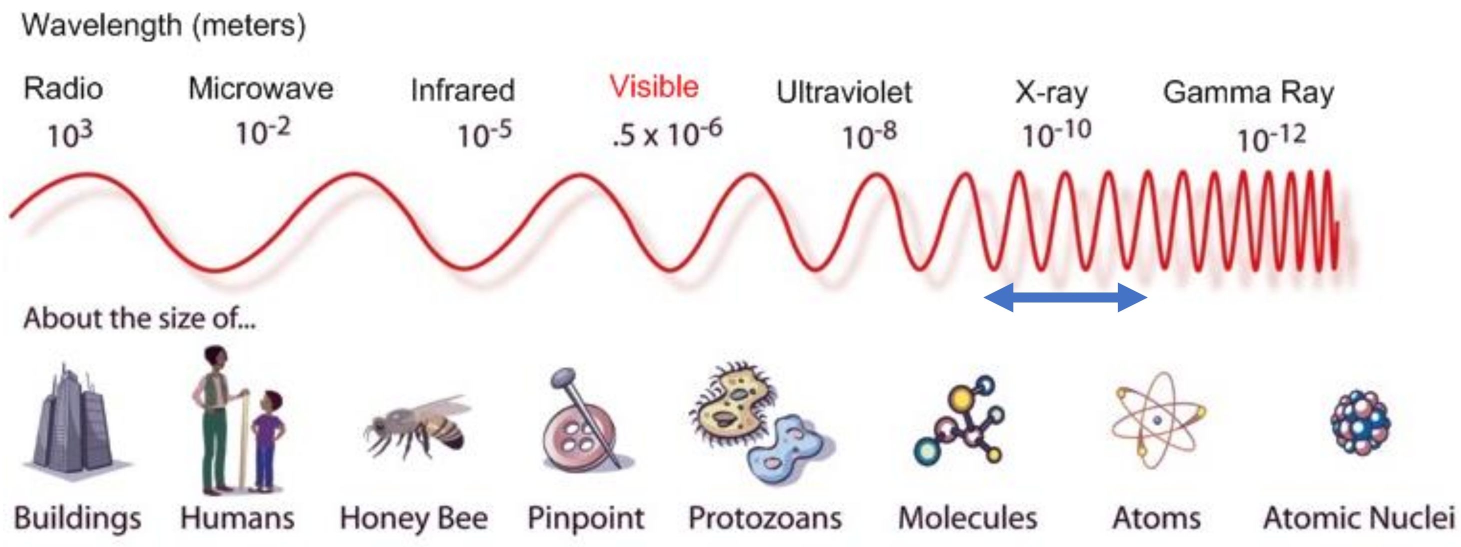
- Tool used to understand the crystallography of the material.
- Understanding of the basic principle involved with the technique (XRD).
- Case studies of XRD.

Why can X-ray be used for diffraction?

- X-radiation ("X-rays") is electromagnetic radiation with wavelengths between ~ 0.1Å and 100 Å, typically like the interatomic distances (~ 2-3 Å) in a crystal. It permits crystal structures to diffract X-rays.

  Lattice parameter of Ni (a_{Ni}) = 3.52 Å
  $\Rightarrow$ d_{hkl} is equal to a_{Ni} or less than that (e.g. $d_{111} = a_{Ni}/\sqrt{3} = 2.03$ Å)

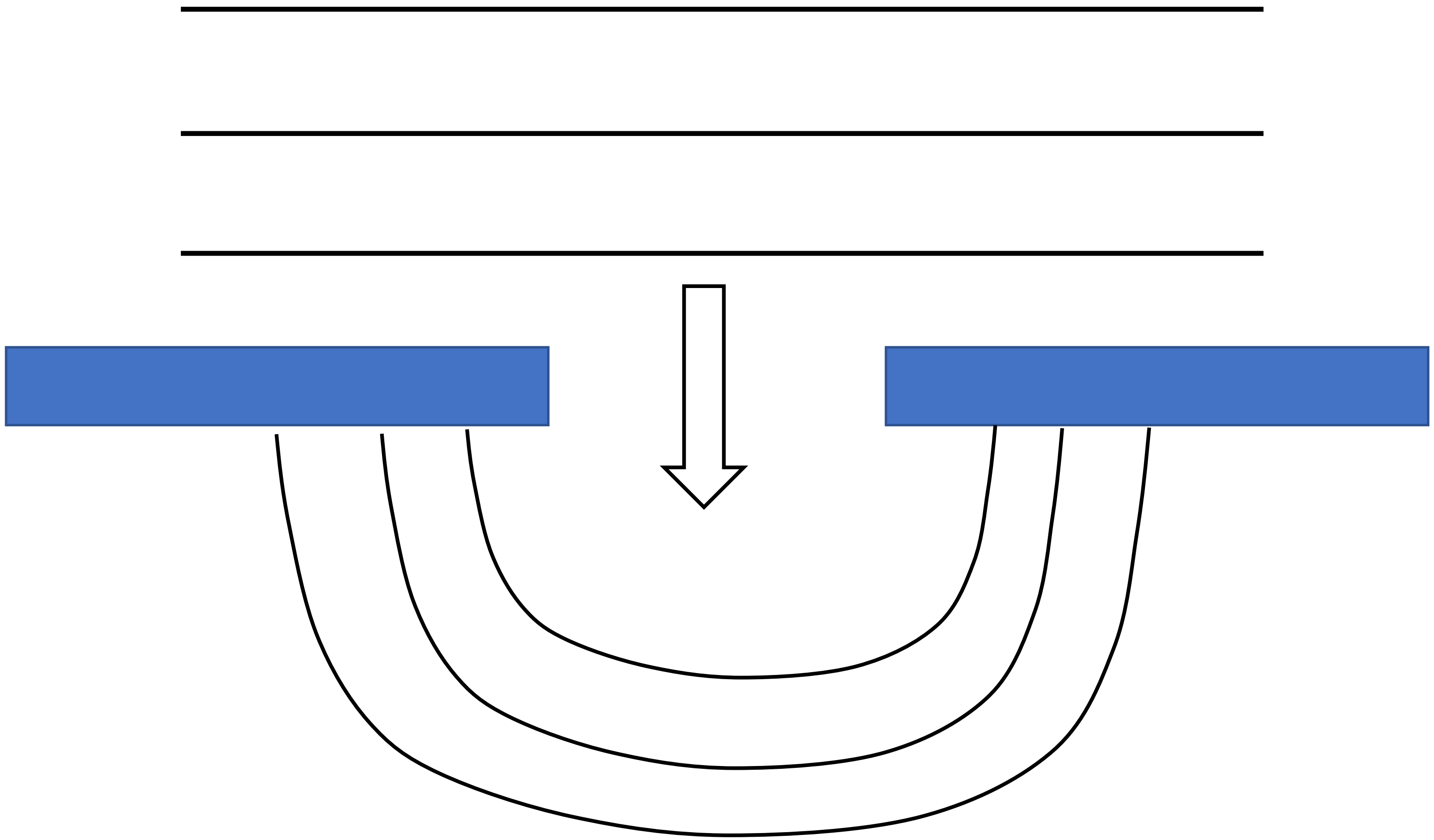
- Three possibilities (regimes) exist based on the wavelength (λ) and the spacing between the scatterers (a).
  - $\lambda < a \rightarrow$ transmission dominated.
  - $\lambda \sim a \rightarrow$ diffraction dominated.
  - $\lambda > a \rightarrow$ reflection dominated (surface phenomenon).



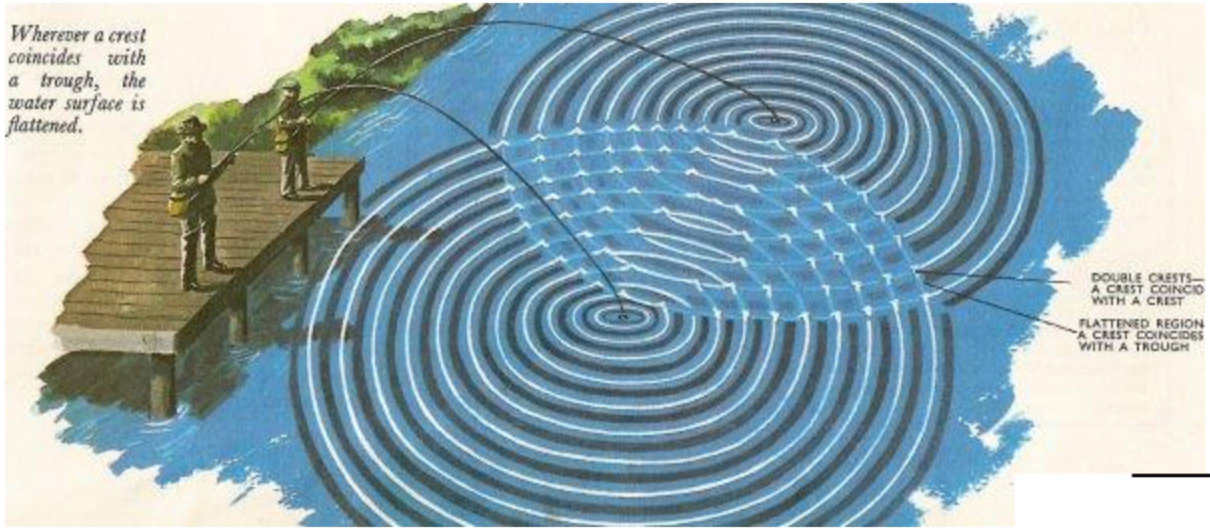
Electromagnetic Spectrum

Diffraction

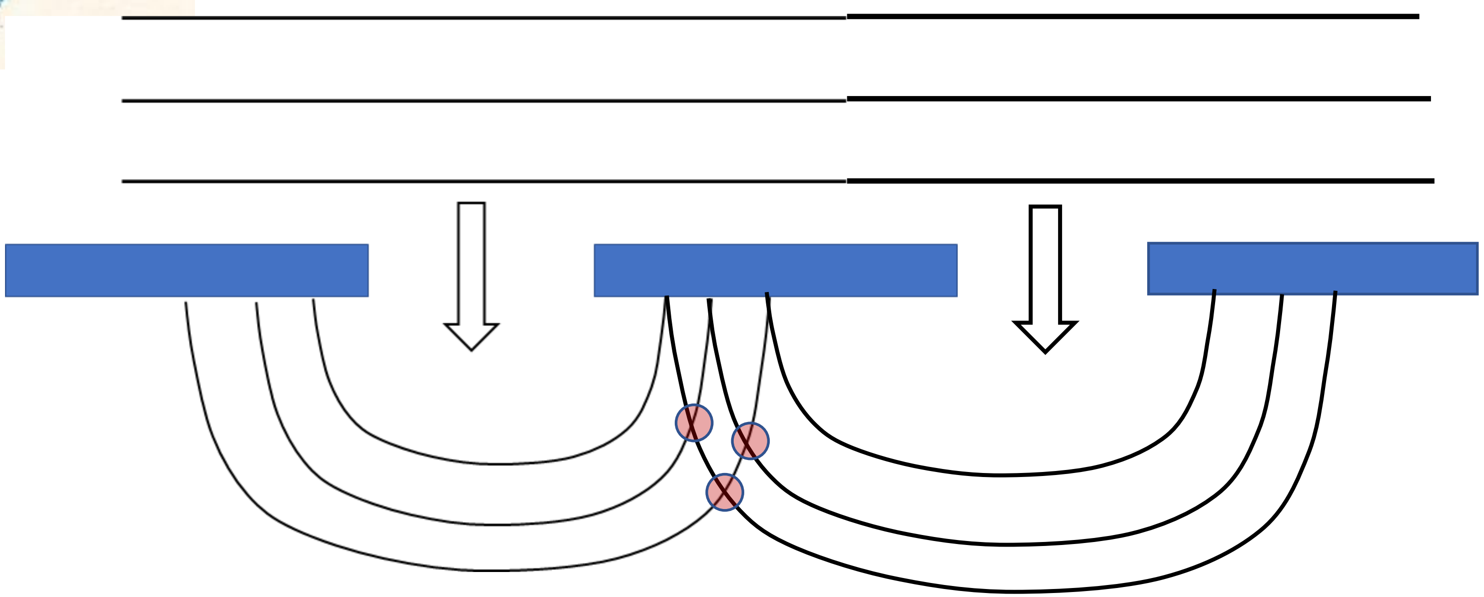
- Series of parallel waves passes through narrow spaces, get constricted, and either spreads out or bends.
- Series of narrowly spaces slits (diffraction grating) disperses parallel beams according to its wavelength.



Interference

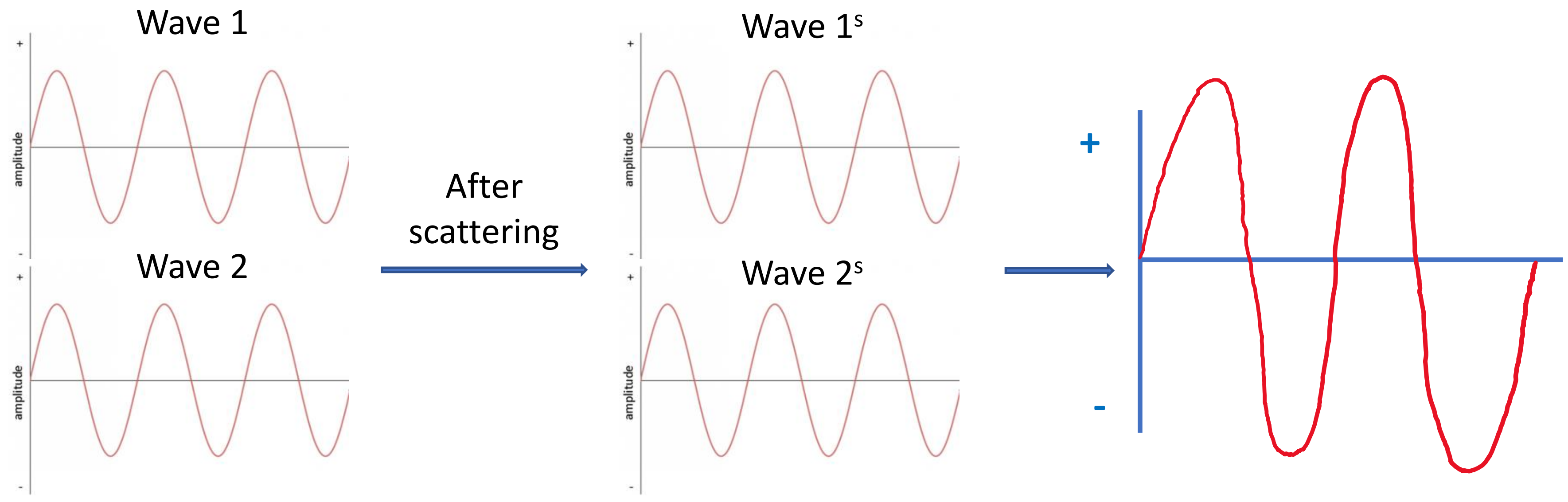


- Two waves encountering each other in the same medium, the effects can either be cancelled out or mutually reinforce each other.

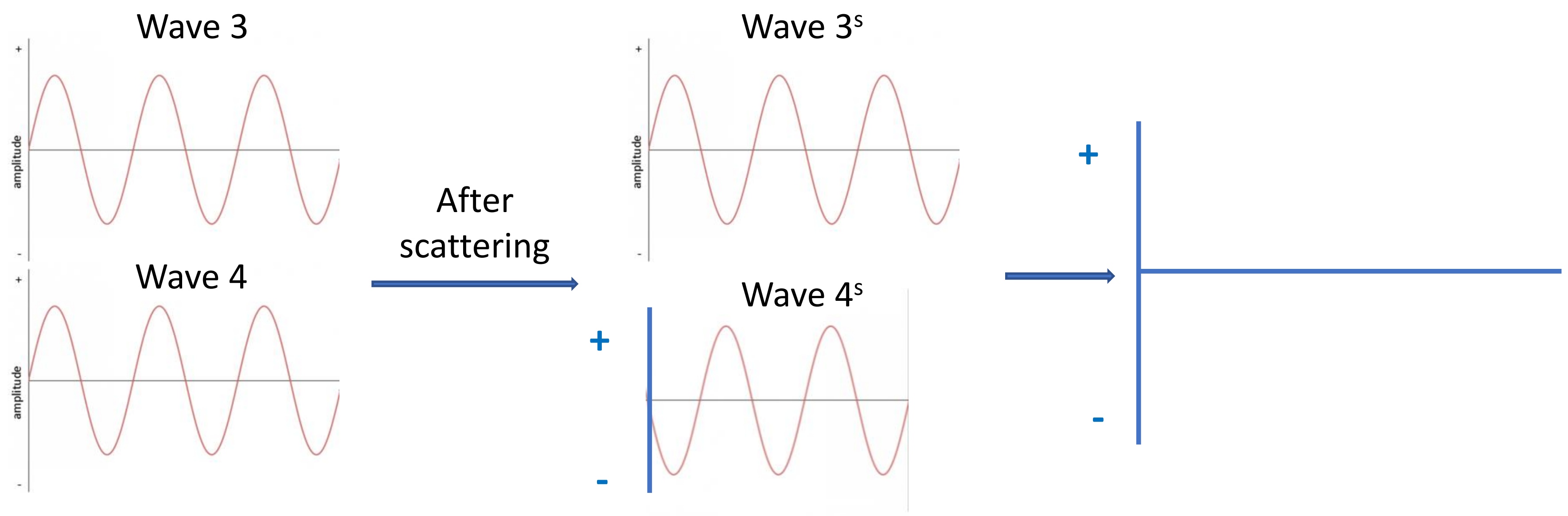


- Amplitude of the disturbance produced by the two combined waves = sum of individual disturbances.

Constructive and Destructive Interference

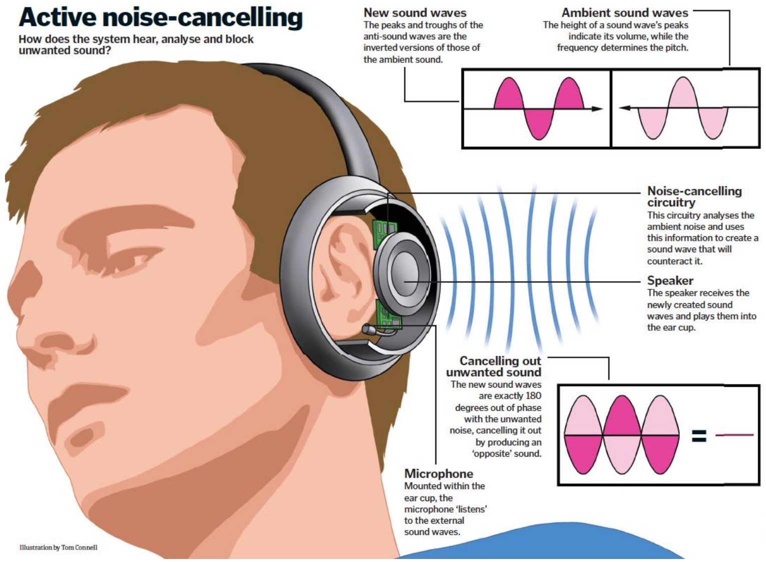


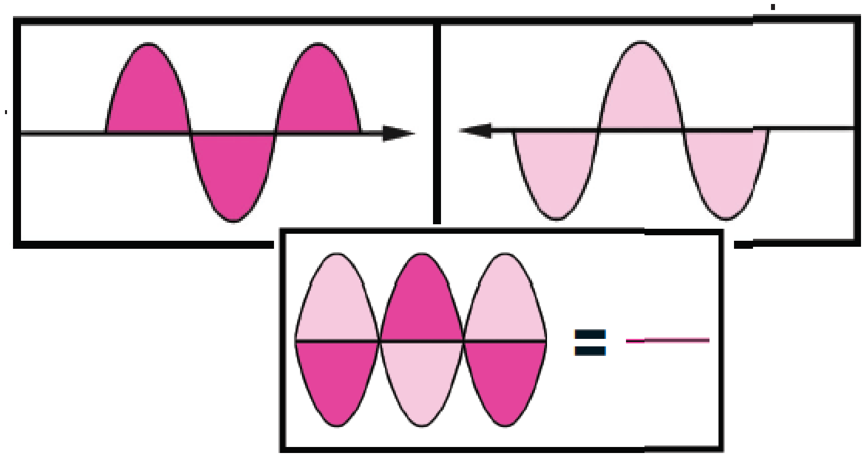
Waves that combine in phase -
---> **Constructive interference**
----> High intensity

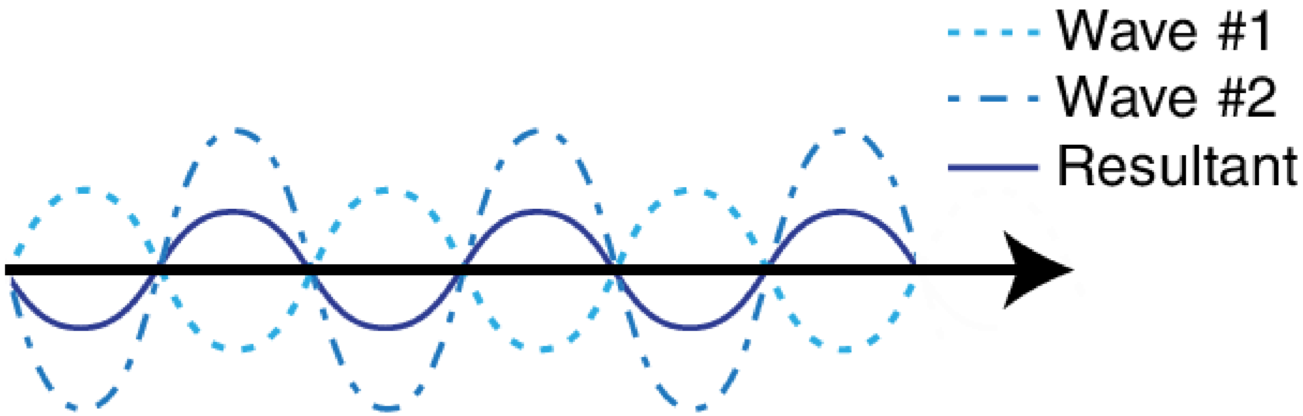


Waves that combine out-of-phase
---->**Destructive interference**
----> Zero intensity

Can something occur in between Constructive and Destructive Interference?

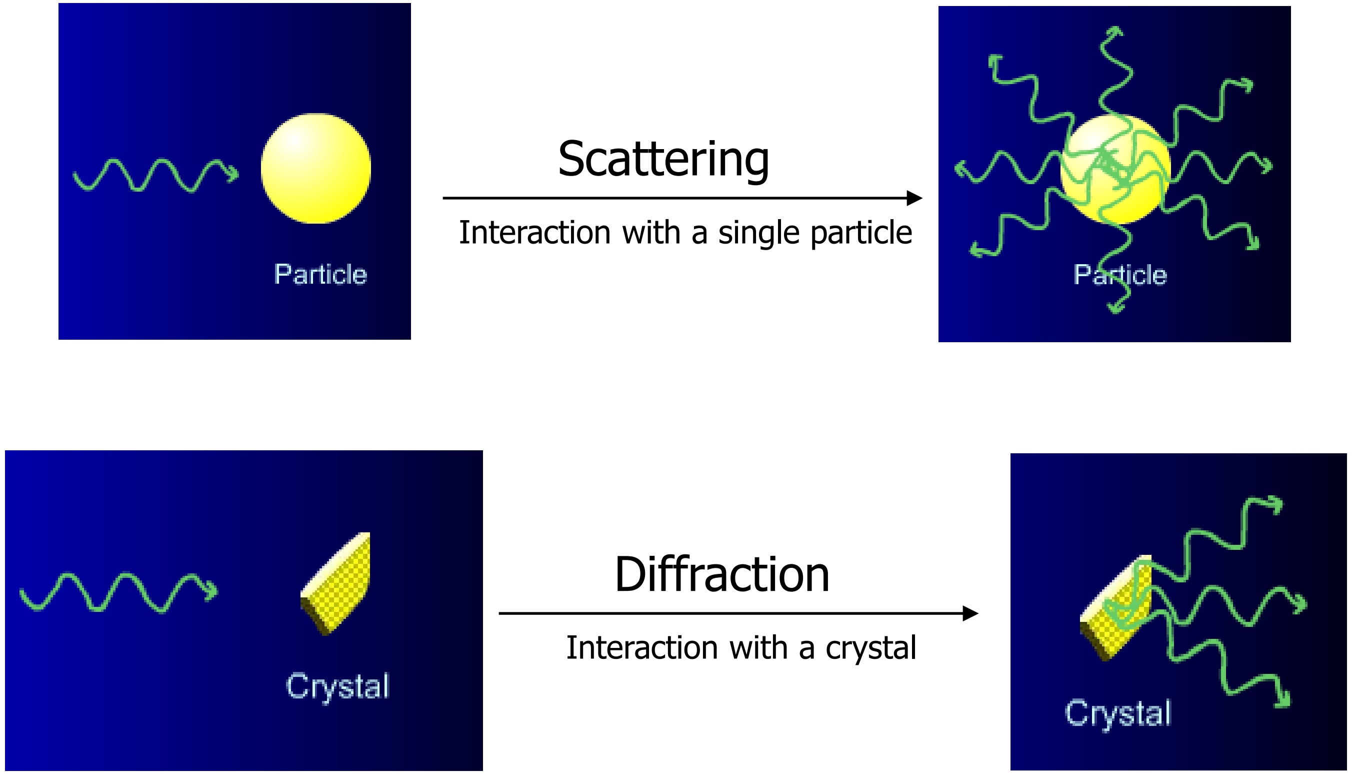






Diffraction in a crystal

A diffracted beam may be defined as a beam composed of many scattered rays mutually reinforcing each other

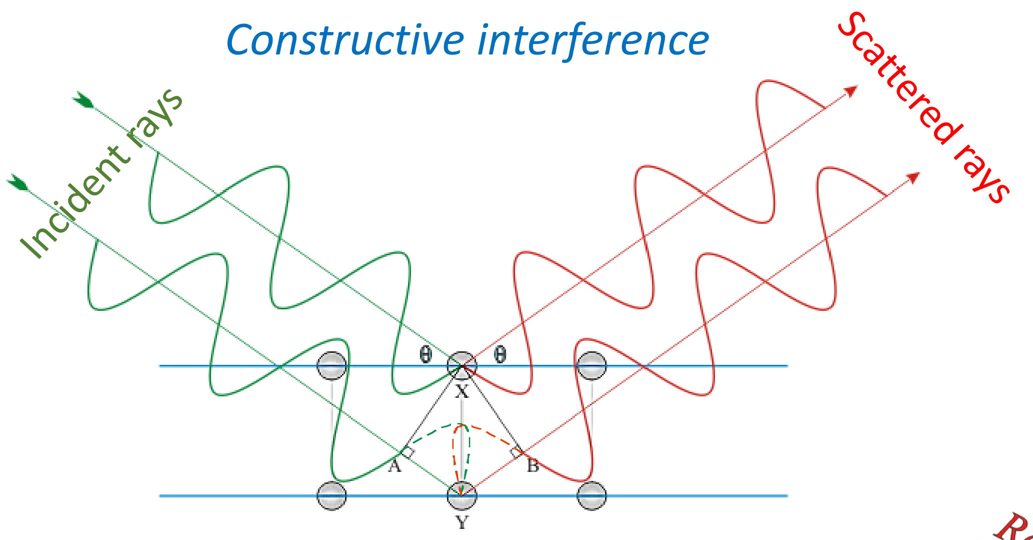


- ❑ **Random arrangement of atoms** in space gives rise to scattering in all directions: weak effect and intensities add.

- ❑ By **atoms arranged periodically** in space
  - ❑ In a few specific directions satisfying Bragg's law: strong intensities of the scattered beam :Diffraction
  - ❑ No scattering along directions not satisfying Bragg's law

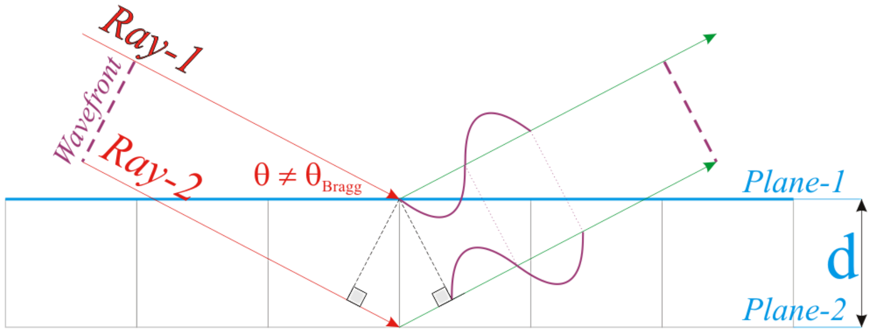
Consider waves scattered from two successive planes interfering constructively

Constructive interference

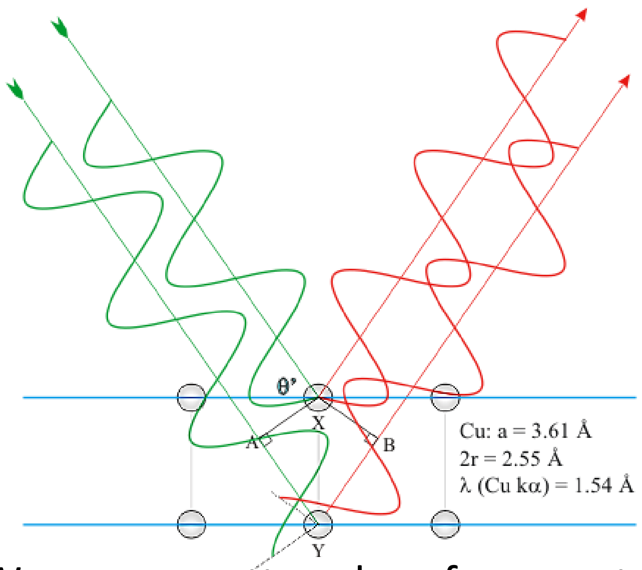


Phase difference of π introduced during the scattering by the atom.

Destructive interference



- Exact destructive interference (between two planes, with path difference of $\lambda/2$).
- The angle is not Bragg's angle.

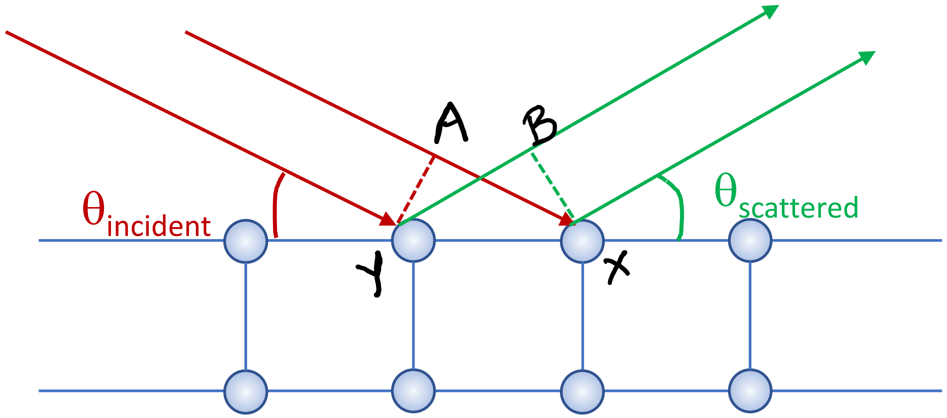


Waves scattered from two successive planes interfere (nearly) destructively at a different angle θ'

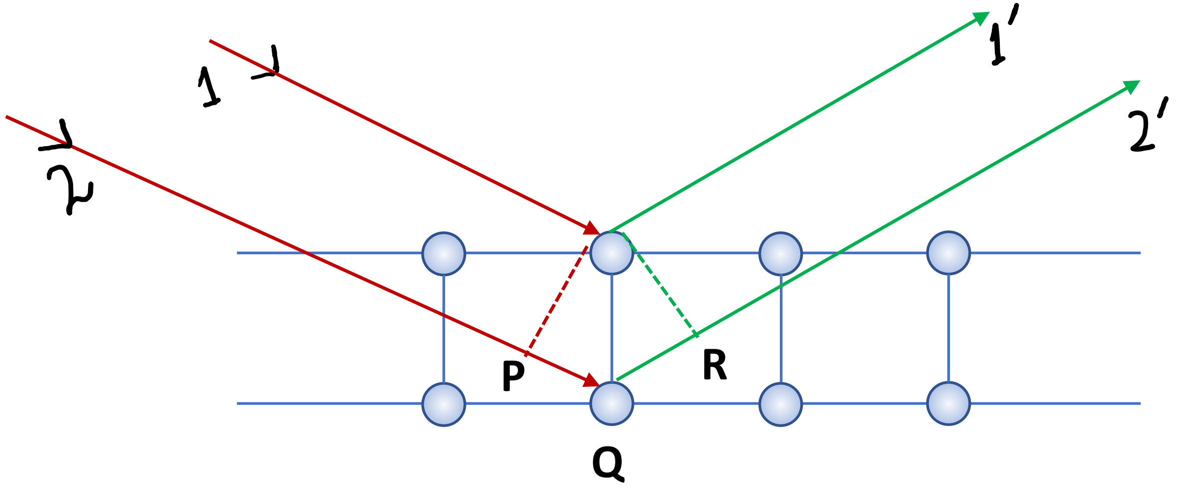
Consider a coherent wave of X-rays impinging on a crystal with atomic planes at an angle θ to the rays.

Incident and scattered waves are in phase if the:

In-plane scattering is in phase



Scattering from across the planes is in phase



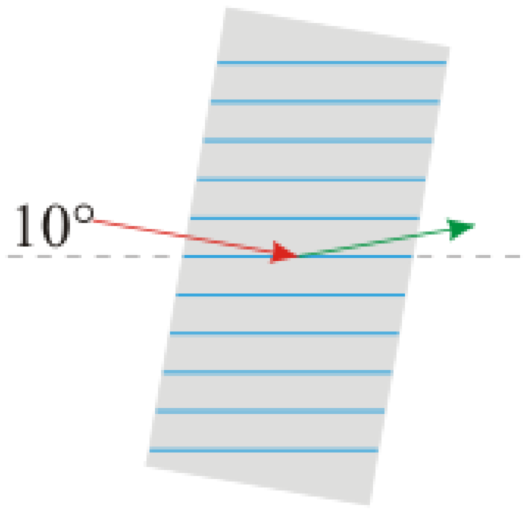
Extra path traveled by incident rays $\rightarrow$ AX

Extra path traveled by scattered rays $\rightarrow$ BY

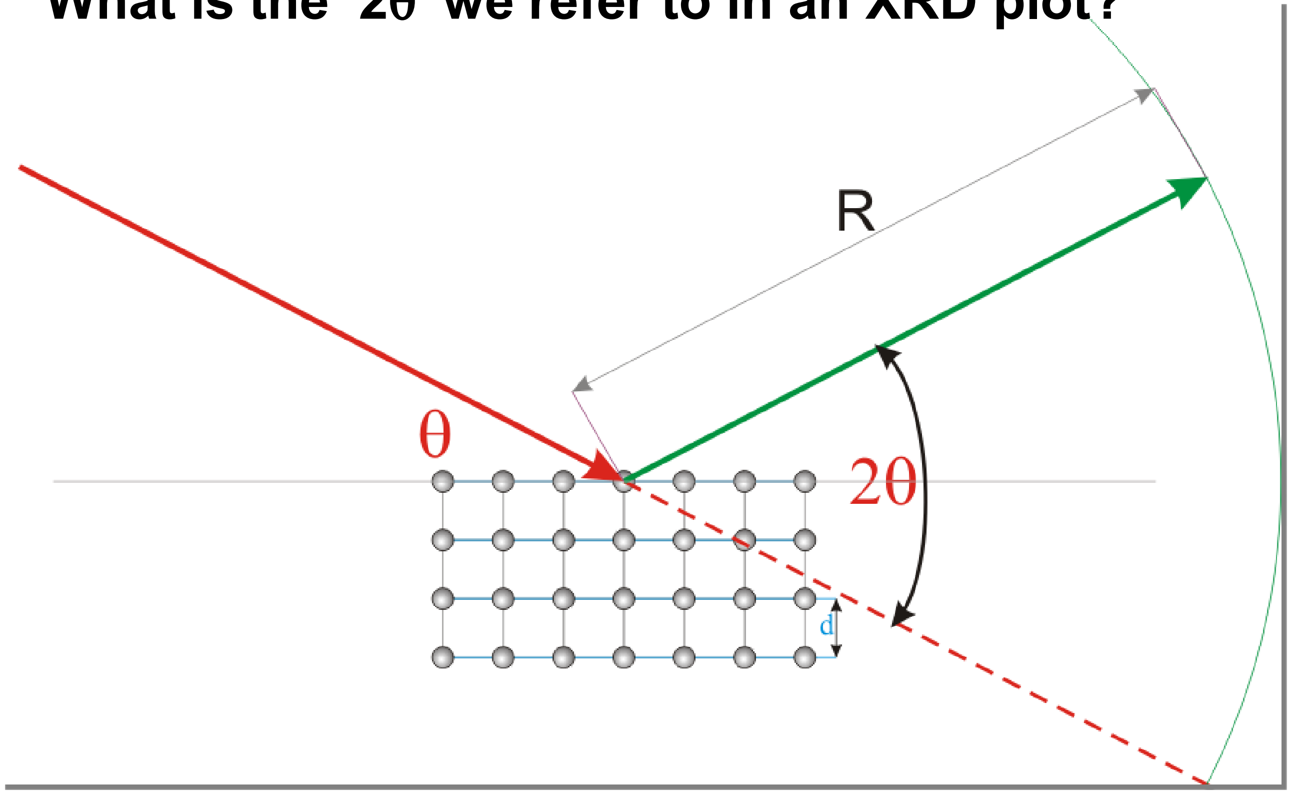
These can be in phase if $\rightarrow$ $\theta_{incident} = \theta_{scattered}$

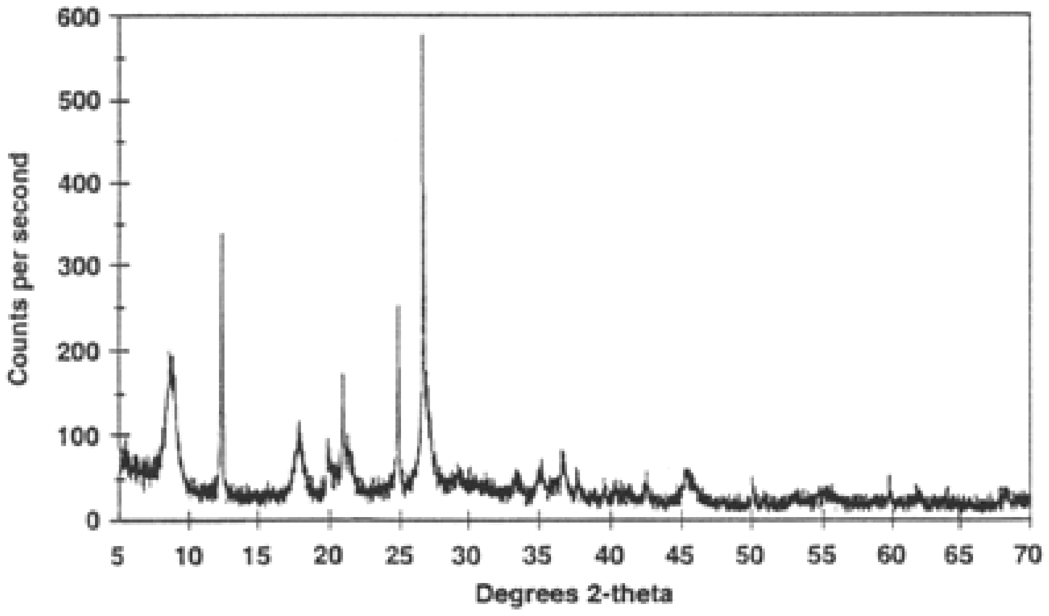
- The scattering planes have an interplanar spacing = ‘d’.
- Ray-2 travels an extra path as compared to Ray-1 (= PQR).
- Path difference between *Ray-1* and *Ray-2* = PQR = (d $\sin\theta$ + d $\sin\theta$) = (2d.$\sin\theta$).
- For constructive interference, this path difference should be an integral multiple of λ: $n\lambda = 2d \sin\theta$ $\rightarrow$ the ***Bragg’s equation***

θ is the angle between the incident x-rays and the set of parallel atomic planes (which have a spacing d_{hkl}).

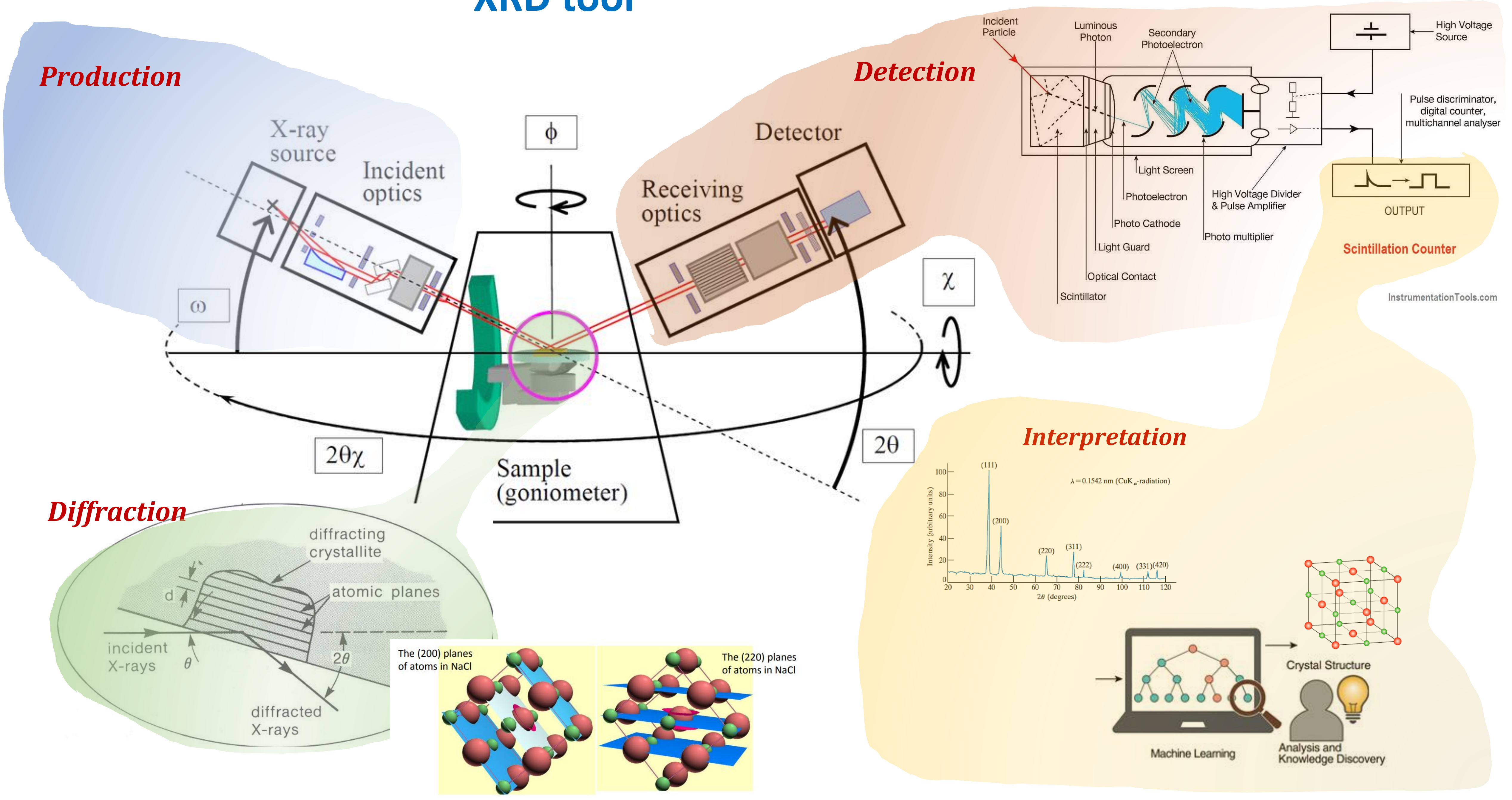


What is the ‘2θ’ we refer to in an XRD plot?





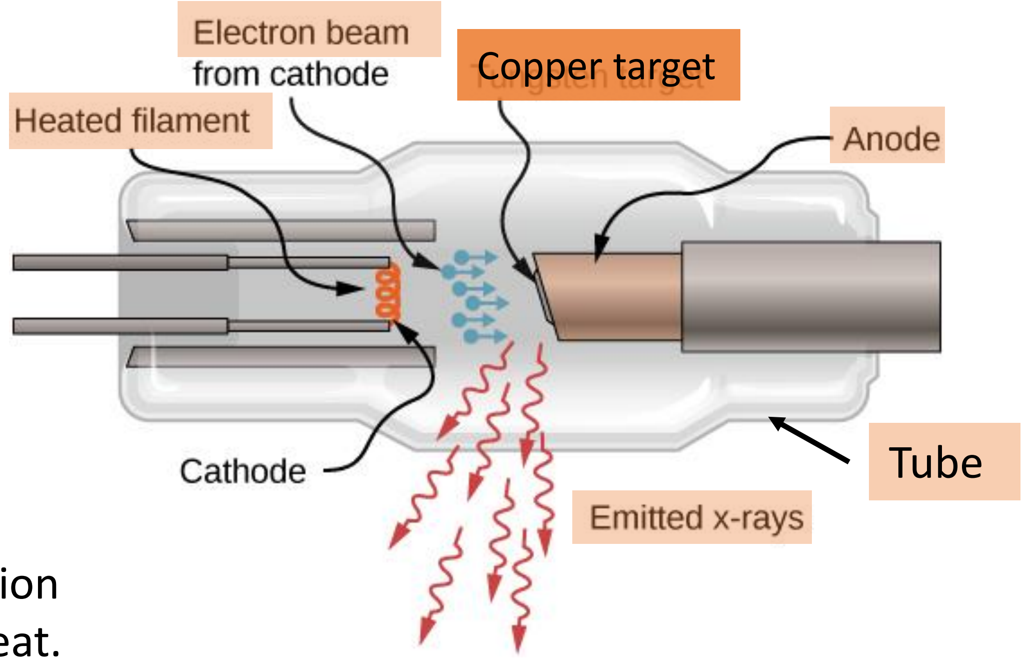
XRD tool


Production
X-ray source
Incident optics
ω
ϕ
Detector
Receiving optics
χ
2θχ
2θ
Sample (goniometer)
Detection
Incident Particle
Luminous Photon
Secondary Photoelectron
High Voltage Source
Pulse discriminator, digital counter, multichannel analyser
Light Screen
Photoelectron
High Voltage Divider & Pulse Amplifier
Photo Cathode
Photo multiplier
Light Guard
Optical Contact
Scintillator
OUTPUT
Scintillation Counter
InstrumentationTools.com
Diffraction
diffracting crystallite
atomic planes
d
incident X-rays
θ
2θ
diffracted X-rays
The (200) planes of atoms in NaCl
The (220) planes of atoms in NaCl
Interpretation
λ = 0.1542 nm (CuKα-radiation)
Intensity (arbitrary units)
2θ (degrees)
(111)
(200)
(220)
(311)
(222)
(400)
(331)
(420)
Crystal Structure
Machine Learning
Analysis and Knowledge Discovery

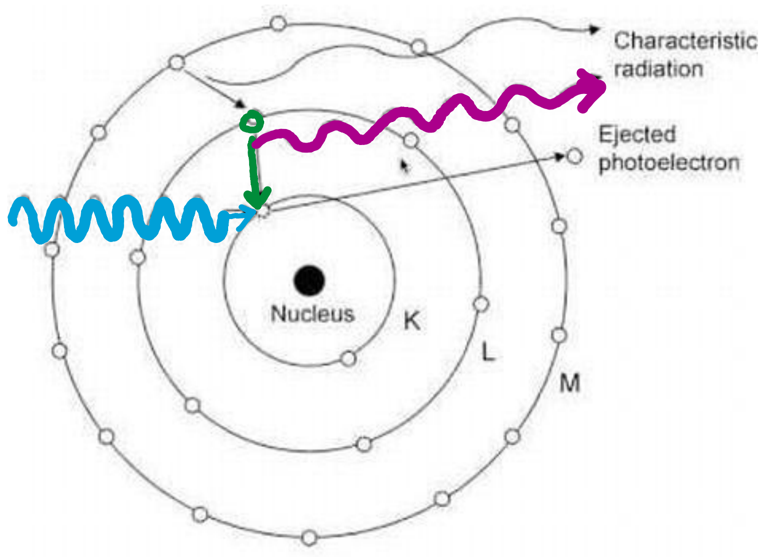
How are X-rays produced?

- *X-rays are produced when high-energy charged particles (electrons) accelerated through very high potential difference (30 kV) collide with matter.*

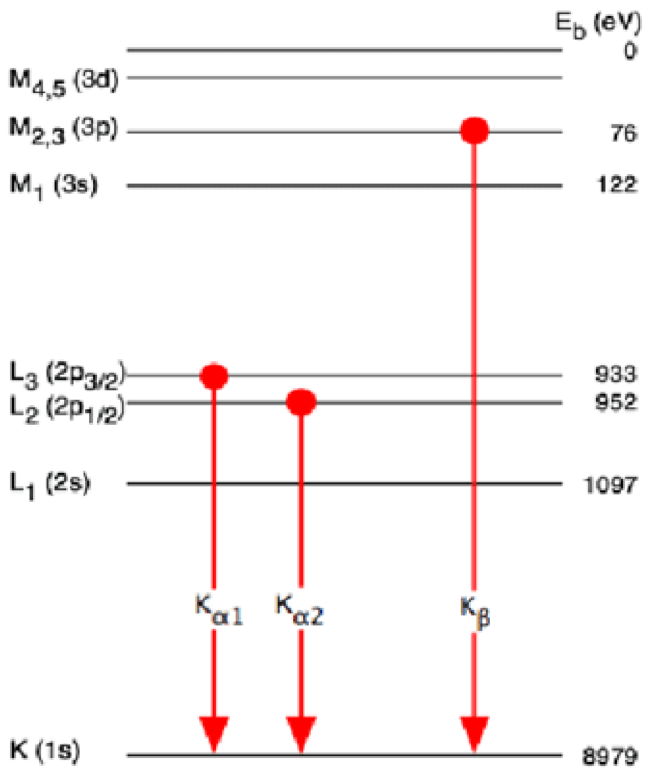
- Laboratory source of X-rays consists of an evacuated tube.
- Electrons are emitted from a heated tungsten filament.
- Electron beam accelerated towards an anode by an electric potential difference of ~ 30 kV to impinge on a water-cooled metal target.
- Electrons strike the Cu target fixed to the anode.
- A spectrum of X-rays get emitted.
- X-rays leave the tube through Be window.



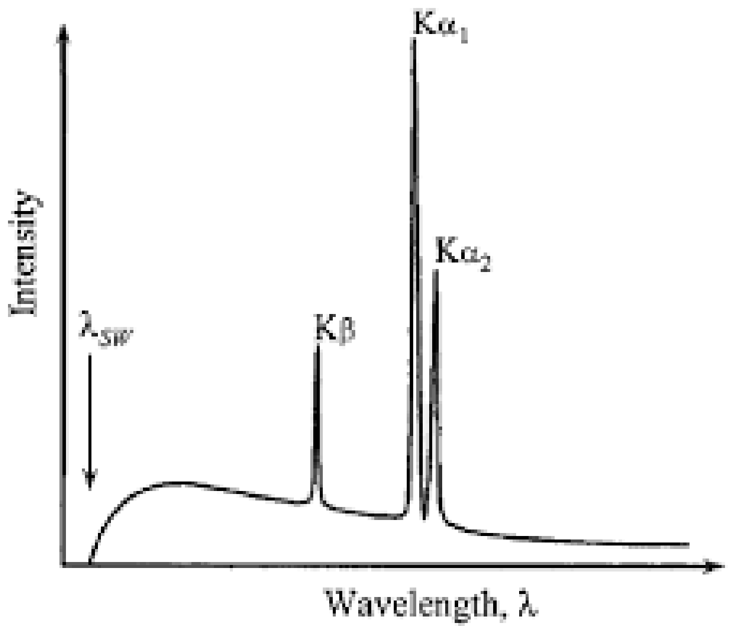
- Continuous cooling of anode is necessitated because only a small fraction of electron energy gets converted to X-ray and rest get converted to heat.



- Incident electrons with sufficient energy ionizes Cu 1s electron.
- An electron from outer orbital (2p or 3p) immediately drops down to the vacant K-level.
- Energy released in the transition appears as X-ray radiation.
- Transition energies have fixed values, so, a spectrum of characteristic X-rays results.
- Consider Cu, 2p ------> 1s transition ($\lambda_{K\alpha}$ = 1.5418 Å) and 3p -----> 1s transition ($\lambda_{K\beta}$ = 1.3922 Å) [K_α is more intense than K_β].



Characteristic X-ray: caused by electronic transitions within an atom



- K_α is a doublet (K_{α_1} = 1.54051 Å, K_{α_2} = 1.54433 Å)
- The 2p ---> 1s has a slightly different energy for the two possible spin states of the 2p electron which makes the transition, relative to the spin of the vacant 1s orbital.
- K_{α_1} and K_{α_2} are not sometimes resolved and appear as a single peak.