X-ray diffraction (XRD)

Chapter 11 from de Graef's book

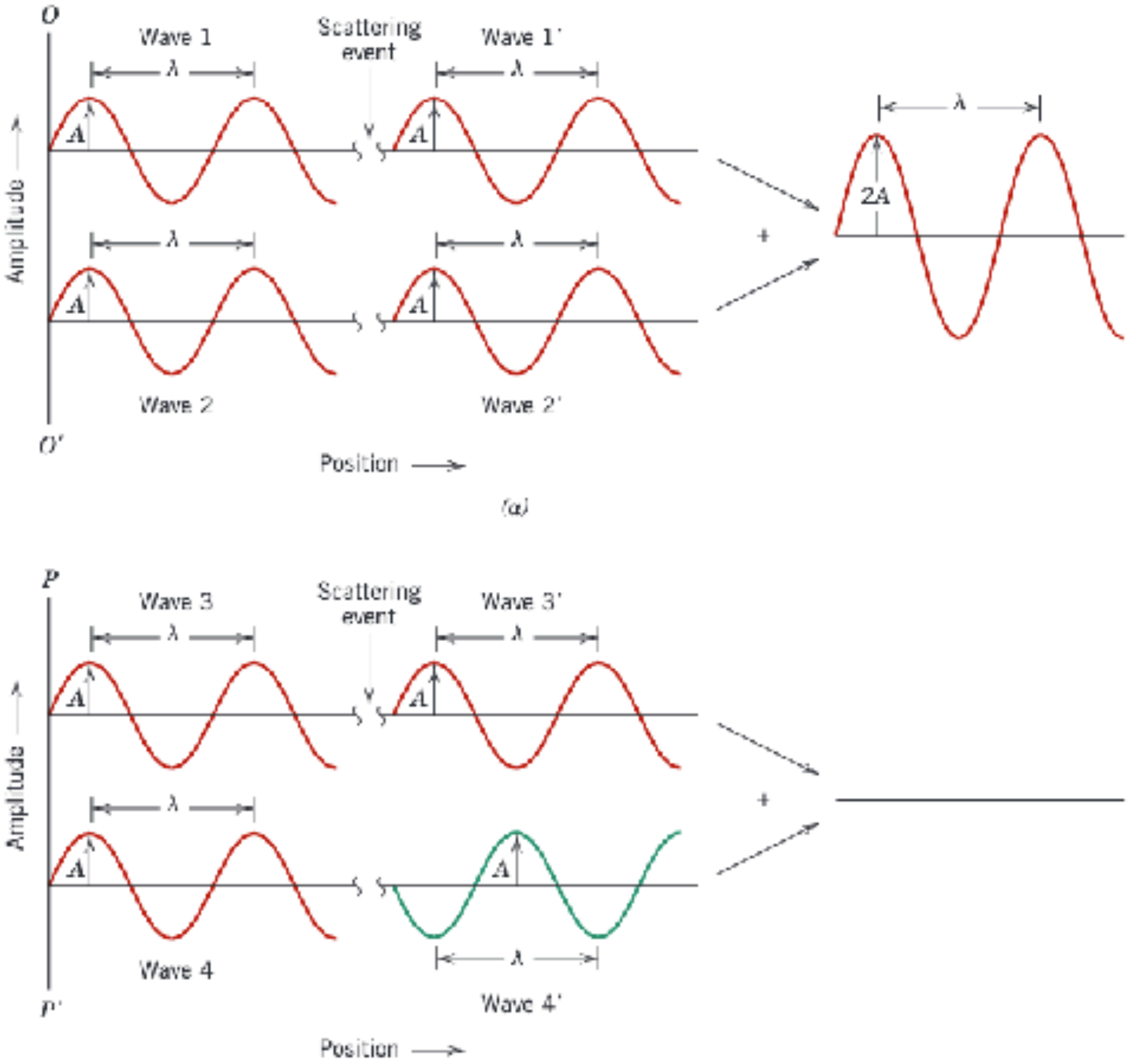
Utility of the technique

- Arrangement of motifs in a lattice
- Positions of atoms in a motif
- Microstructure of the material
- Deformation of the lattice
- … and many other things

Phenomenon of diffraction

- Regularly spaced obstacles
  - Scatter an EM wave
  - Spacing comparable to wavelength of radiation

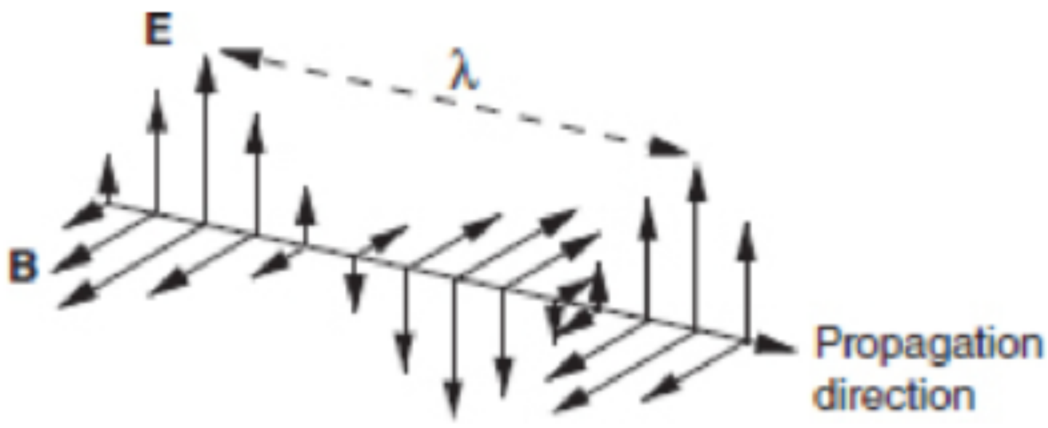
- Phase relationships between adjacent events



X-rays: characteristics

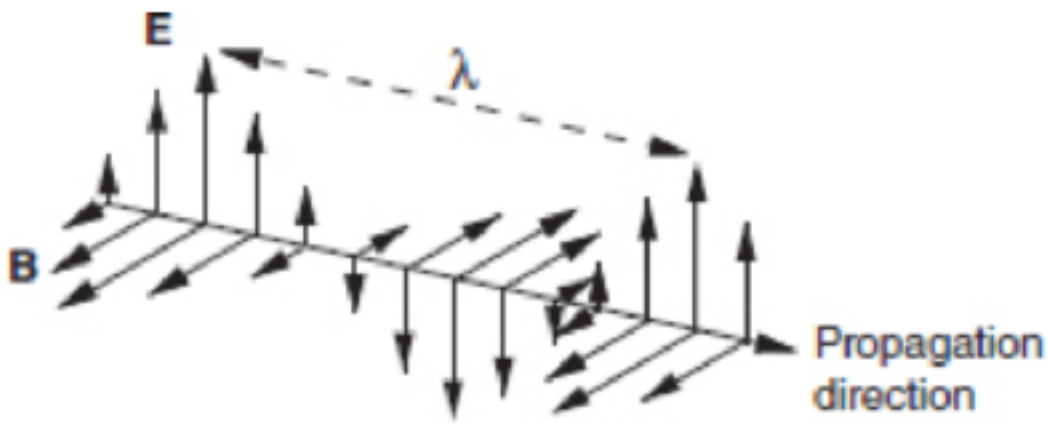
- short wavelength EM radiation with high energies (100 eV to 100 keV)
- wavelength ~ 0.01 to 10 nm
- atomic spacing: Cu – 0.36 nm; Al – 0.148 nm; Fe – 0.23 nm; Au – 0.407 nm

X-ray wavenumber



- $E(x,t) = A\exp(2\pi i k(x - ct))$
  - $k \rightarrow$ wavenumber
  - only real part has physical meaning
- $E(x,t) = A\exp 2\pi i k x$
  - temporal variation can be omitted
- argument of an exponential function must be dimensionless $\Longrightarrow$ the dimensions of the wavenumber k are the inverse of length

X-ray wavenumber



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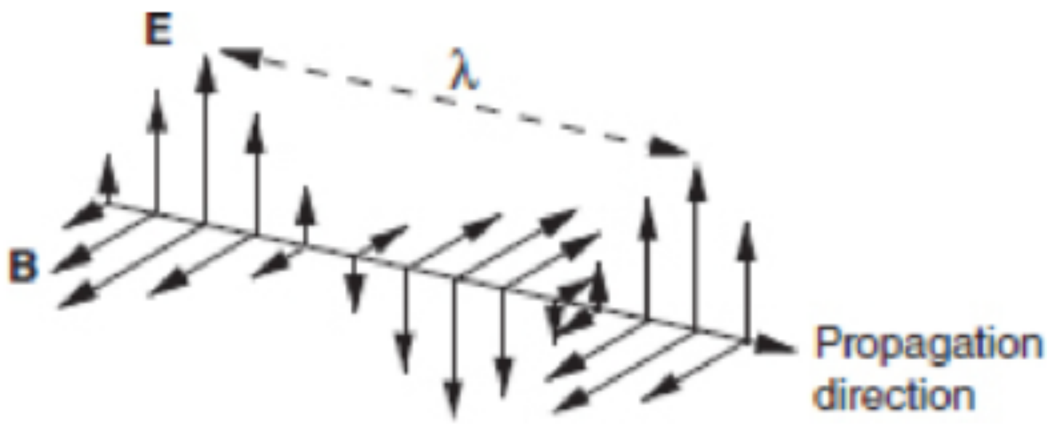
***k* is therefore, a vector in reciprocal space**

X-ray as plane waves



- Consider arbitrary propagation direction

- $E(\mathbf{r}, t) = A \exp 2\pi i\ \mathbf{k} \bullet \mathbf{r}$
  - $\mathbf{k} = k_i \mathbf{a_i^*}$; $\mathbf{r} = x_i \mathbf{a_i}$
  - $\mathbf{k} \bullet \mathbf{r} = k_i x_i$

- $\mathbf{k} \bullet \mathbf{r} = k_i x_i$ will be constant in a plane to which the propagation direction is perpendicular

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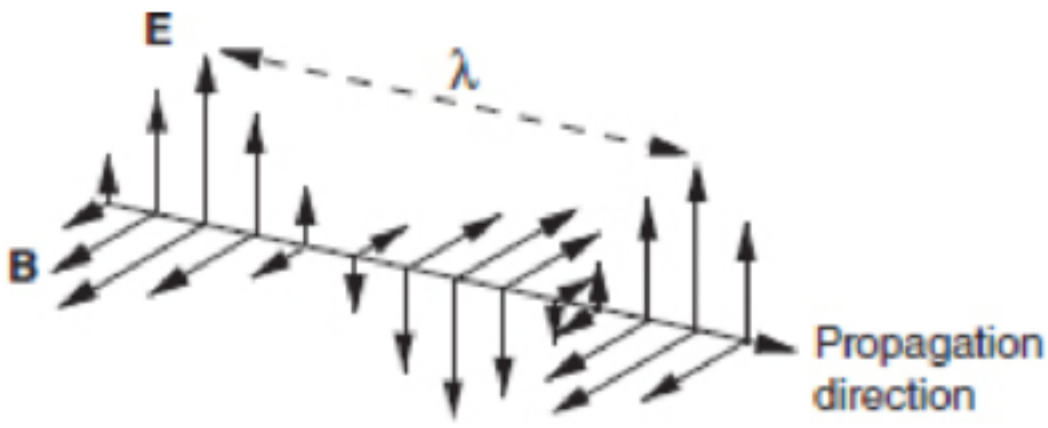

It is for this reason that waves described by this expression are termed ***plane waves***

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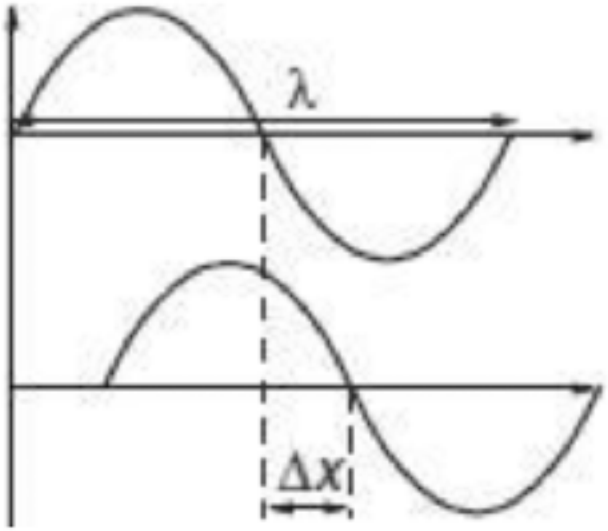
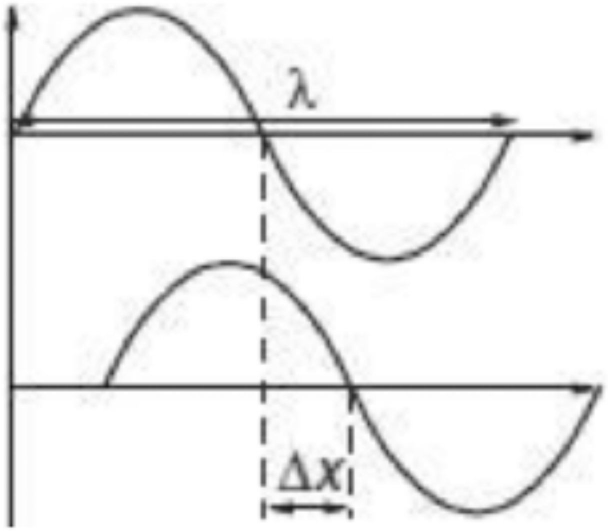
Phase difference



- Consider two periodic waves with wavelength λ, but shifted with respect to each other
  - define origin as point at which the first wave has zero amplitude
  - $\Delta x \rightarrow$ distance to the closest zero crossing of the second wave
  - Multiply this distance by $\dfrac{2\pi}{\lambda} \rightarrow \phi$, the phase difference

Phase difference



phase shifted wave can be represented by the addition of ϕ to the argument

$$\rightarrow A\cos\left(\frac{2\pi x}{\lambda}+\phi\right)$$

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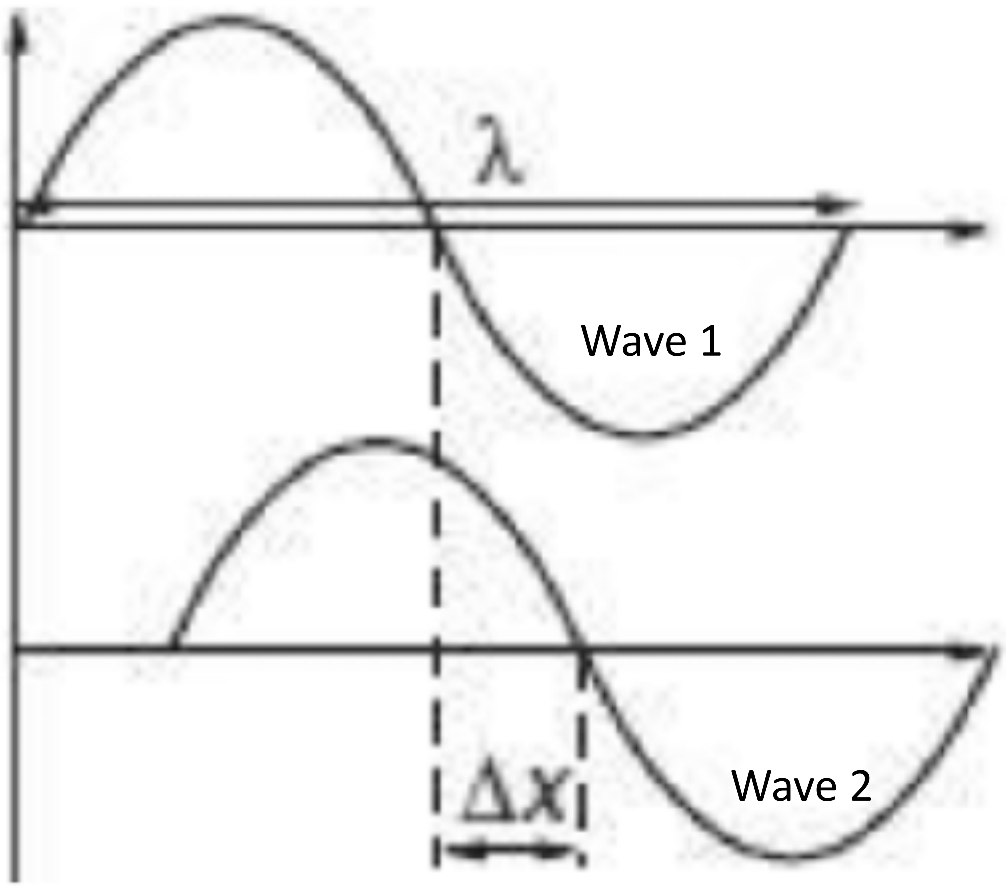
Interference of phase-shifted waves



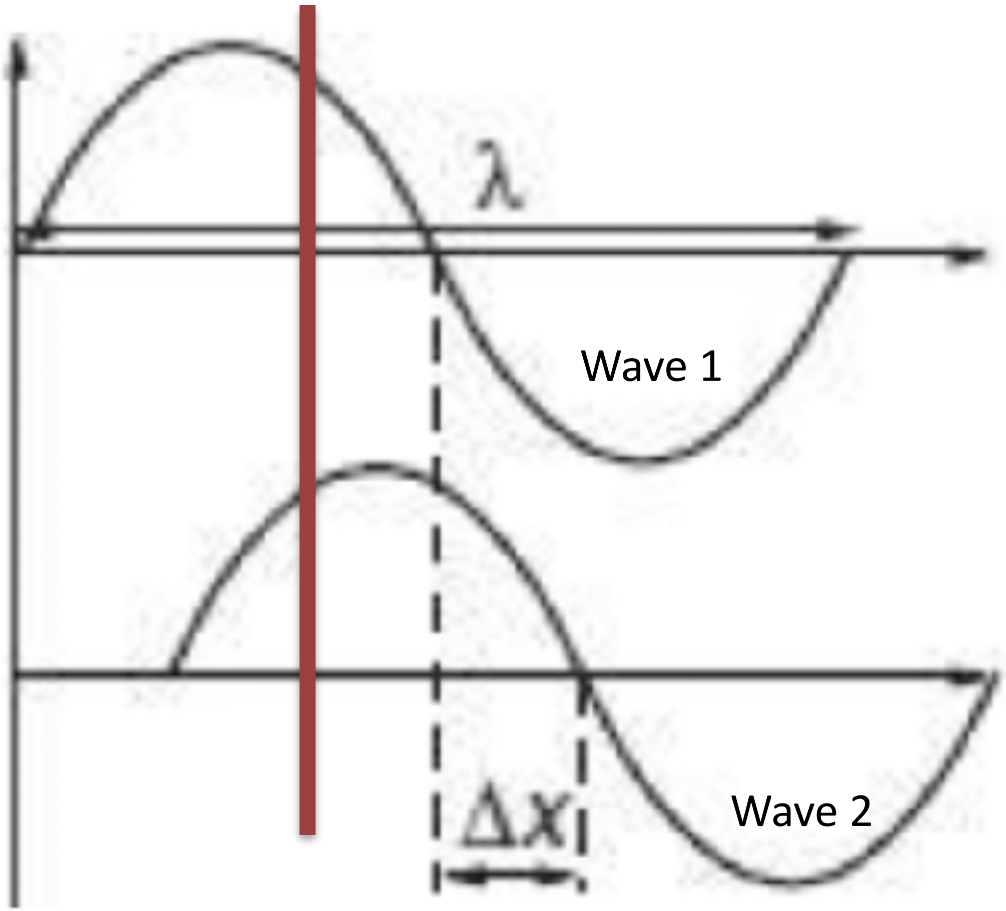
- What is the amplitude at a specific position, x, due to both waves propagating in the medium

- Sum of the amplitudes of individual waves

$$\rightarrow 2A\cos\left(\frac{2\pi x}{\lambda}+\frac{\phi}{2}\right)\times\cos\frac{\phi}{2}$$

- Destructive interference when $\phi = 180^{\circ}$

Interference of phase-shifted waves



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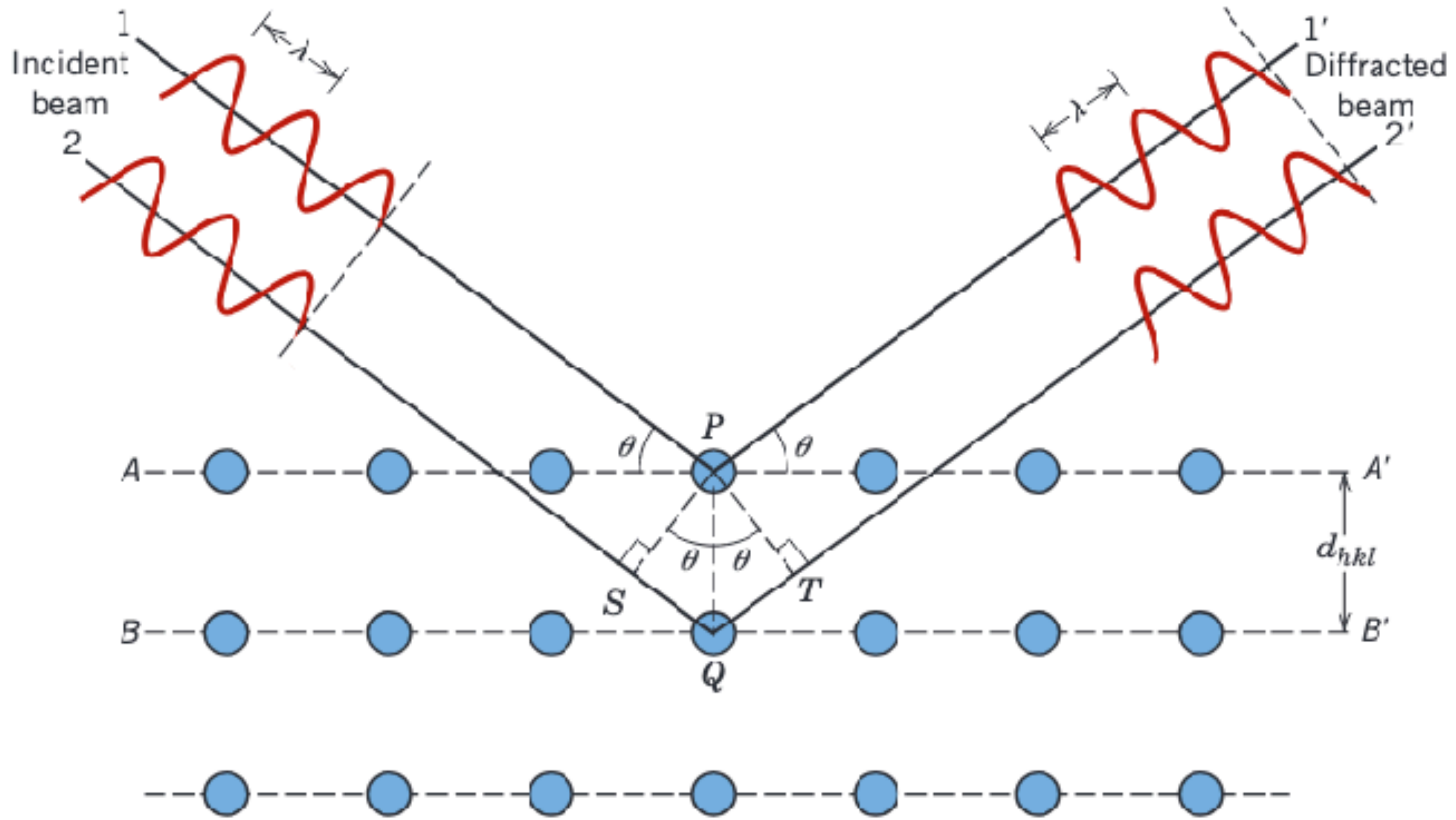
X-ray diffraction from a crystal: phase difference from path length difference



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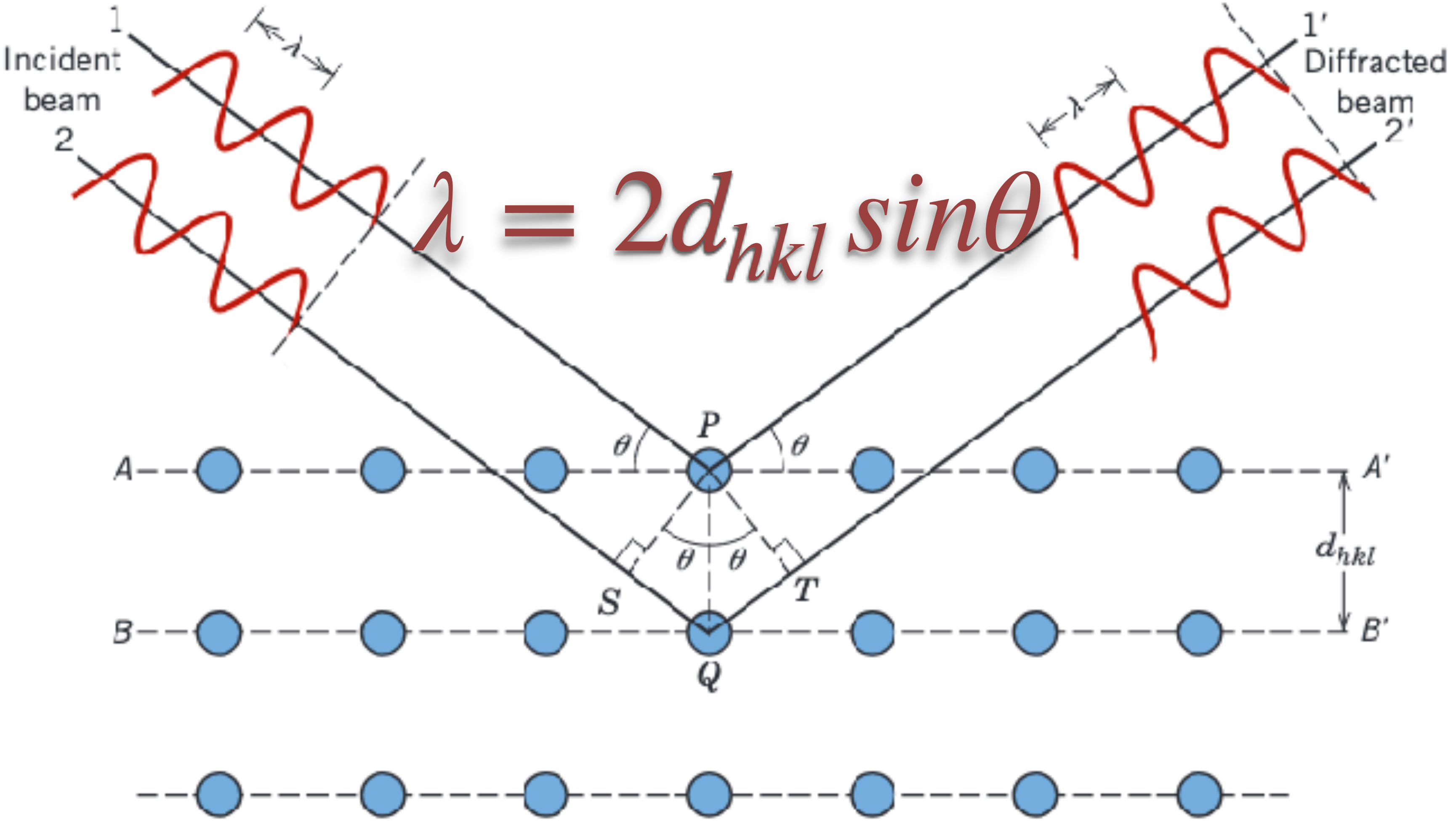

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$$2\theta = 2 \times \arcsin \left\{ \begin{array}{c} \dfrac{\lambda \times \sqrt{1}}{2 \times a} \\ \dfrac{\lambda \times \sqrt{2}}{2 \times a} \\ \vdots \end{array} \right\}$$

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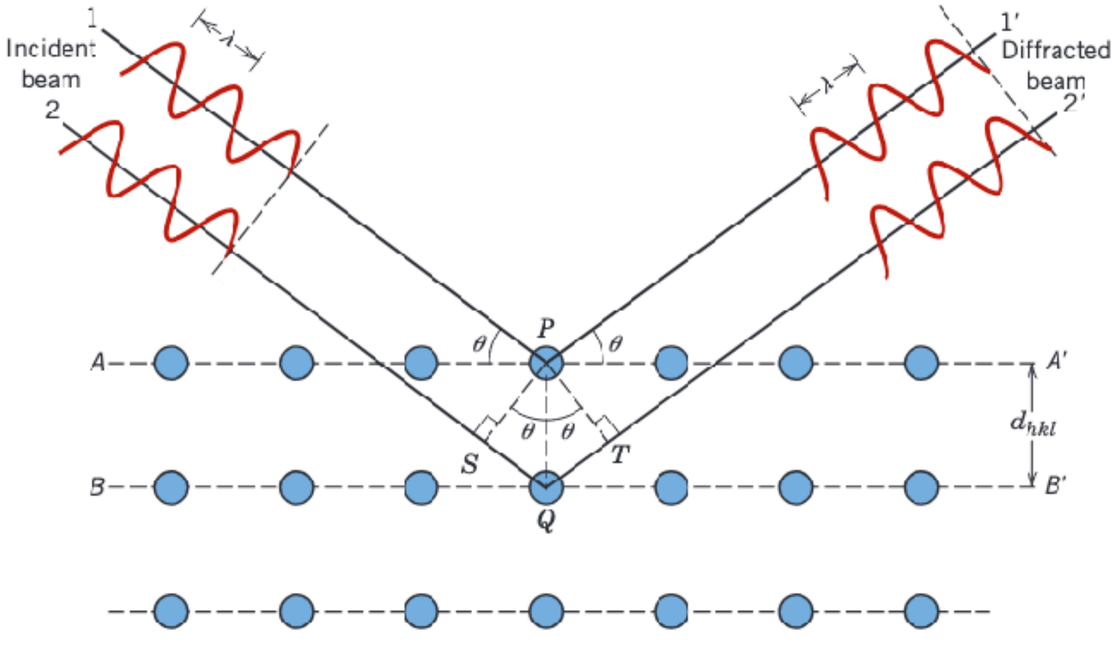

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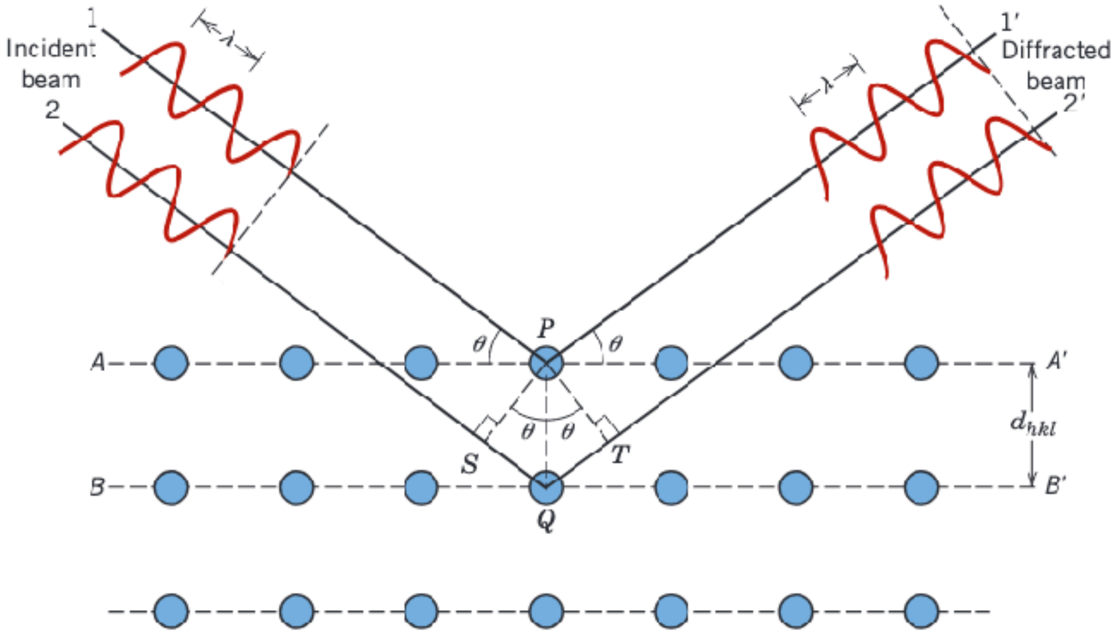

$$\lambda = 2d_{hkl}\, sin\theta$$

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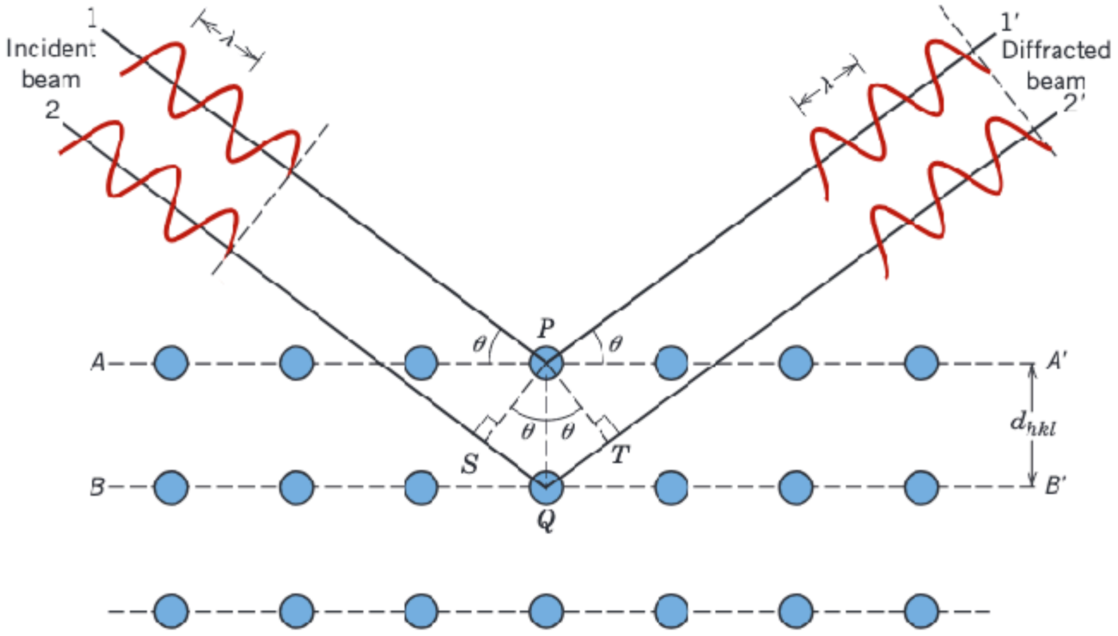

$$\lambda = 2d_{hkl}\, sin\theta$$

$$d_{hkl} = \left[\begin{pmatrix} h & k & l \end{pmatrix} g^*_{ij} \begin{pmatrix} h \\ k \\ l \end{pmatrix} \right]^{-\frac{1}{2}}$$

Problem

For BCC iron, compute :

(a) the interplanar spacing
(b) the diffraction angle for the (220) set of planes.

The lattice parameter for Fe is 0.2866 nm. Also, assume that monochromatic radiation having a wavelength of 0.179 nm is used.

Problem

Cu K-alpha radiation with $\lambda = 1.54054$ Å is used to examine materials.

- Given atomic radius of Pt is 0.1387 nm, and that it crystallises in a fcc structure, determine the expected diffraction angle for the second-order reflection from the (113) set of planes
- Given that Ir has an FCC crystal structure and angle of diffraction for the (220) set of planes occurs at 69.22°, determine the atomic radius of Ir