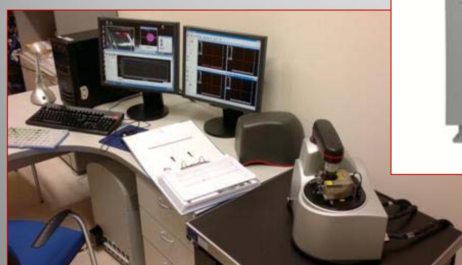


PHYS485

Materials Physics

Dr. Gregory W. Clark
Manchester University

Symmetry Operations

- Matrix representation: a few examples

Identity

$$E = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Inversion

$$I = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

Rotation

rotation about the *z*-axis

$$C_n = \begin{pmatrix} \cos 2\pi/n & \sin 2\pi/n & 0 \\ -\sin 2\pi/n & \cos 2\pi/n & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Reflection

$$\sigma_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

reflection in *x*-*y* plane

$$\sigma_x = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

reflection in *y*-*z* plane

Rotary-reflection

rotation about the *z*-axis then reflection in *x*-*y* plane

$$S_{nz} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} \cos 2\pi/n & \sin 2\pi/n & 0 \\ -\sin 2\pi/n & \cos 2\pi/n & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} \cos 2\pi/n & \sin 2\pi/n & 0 \\ -\sin 2\pi/n & \cos 2\pi/n & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

Symmetry Operations

- Matrix representation: a few examples

Rotation

rotation about the *x*-axis

$$C_{nx} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos 2\pi/n & \sin 2\pi/n \\ 0 & -\sin 2\pi/n & \cos 2\pi/n \end{pmatrix}$$

Rotation

rotation about the *y*-axis

$$C_{ny} = \begin{pmatrix} \cos 2\pi/n & \sin 2\pi/n & 0 \\ 0 & 1 & 0 \\ 0 & -\sin 2\pi/n & \cos 2\pi/n \end{pmatrix}$$

Rotation

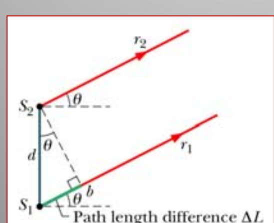
rotation about the *z*-axis

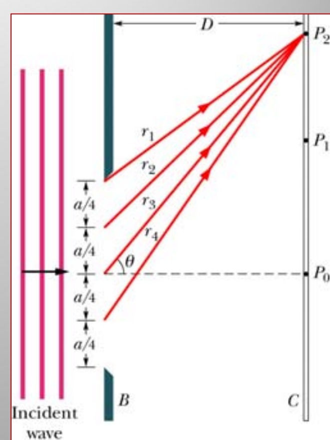
$$C_{nz} = \begin{pmatrix} \cos 2\pi/n & \sin 2\pi/n & 0 \\ -\sin 2\pi/n & \cos 2\pi/n & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Scattering

- Multiple slit diffraction:
  - Constructive interference

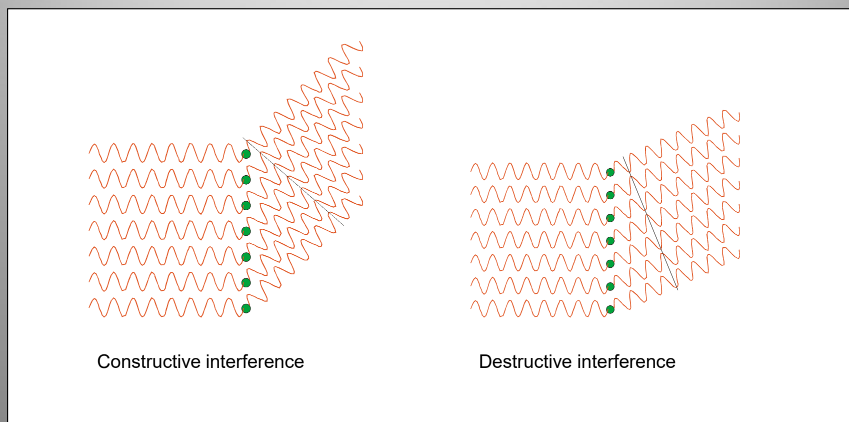
$$d \sin\theta = n\lambda$$





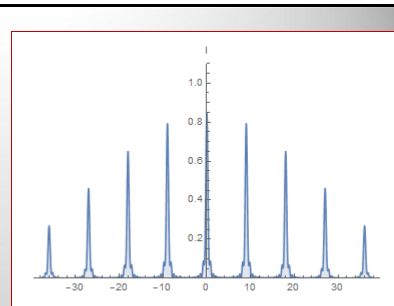
Scattering

- Multiple slit diffraction:



Scattering

- Multiple slit diffraction:

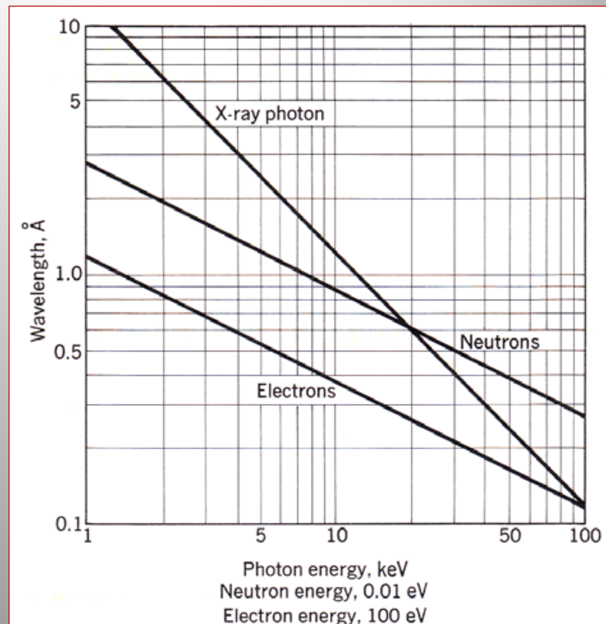


- Intensity of peaks is given by

$$I = 4I_o\left[\frac{\sin\left(\frac{\pi a}{\lambda}\sin\theta\right)}{\frac{\pi a}{\lambda}\sin\theta}\right]^2\left[\sum_{p=1}^{N/2}\cos\left((2p-1)\frac{\pi d}{\lambda}\sin\theta\right)\right]^2$$

where d = distance between slits, a = slit size, N = number of slits

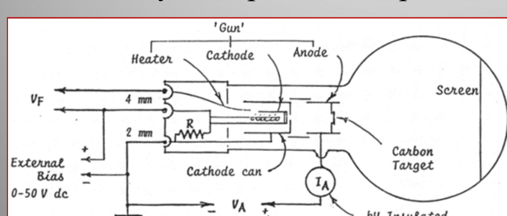
- Possible probes at the atomic level?



Electron Diffraction

- Electrons:
  - ➢ low mass
  - ➢ relatively low energies with appropriate λ

  ∴ very little penetration power



electrons transmitted through sample: acts like a diffraction grating

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

- de Broglie wavelength of a particle:

$$\lambda = \frac{h}{p}$$

where
h ≡ 6.63 x 10^{-34} Js

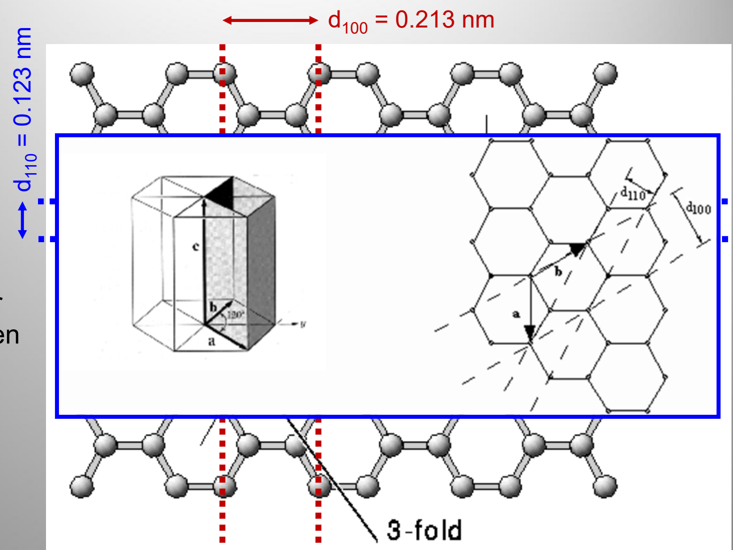
Planck's constant

and $p = m\,v$

Electron Diffraction

- Graphite lattice
- Diffraction caused by spacing within the plane rather than between planes – why?

Transmission!

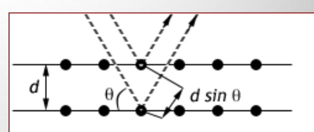


Bragg Scattering

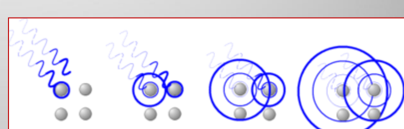
- X-ray diffraction:
  - ➢Bragg's Law: constructive interference

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

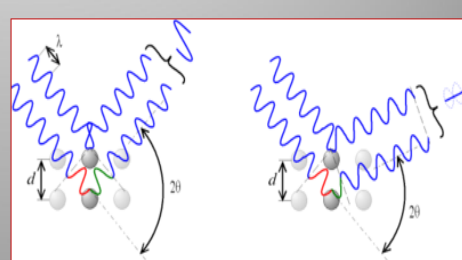
  - ➢Actually, quite general!



Bragg formulation

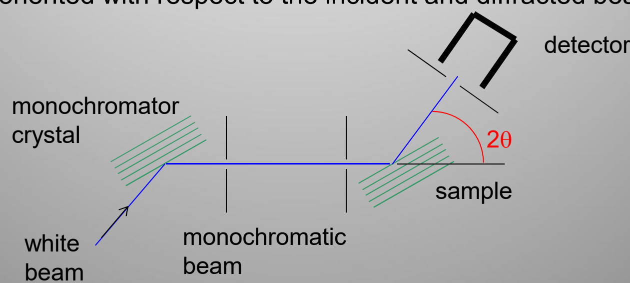


Laue formulation



Diffraction experiments

- **Requirements:**
  - a monochromatic beam (well-collimated)
  - a detector that can scan
  - a way of aligning the crystal so that the selected Miller planes are oriented with respect to the incident and diffracted beams



Reciprocal Lattice Vectors

- Look at the vectors, $\vec{G}$
- Construct axis vectors of the reciprocal lattice:

$$\vec{b}_1 = \frac{2\pi\,\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} \qquad \vec{b}_2 = \frac{2\pi\,\vec{a}_3 \times \vec{a}_1}{\vec{a}_2 \cdot (\vec{a}_3 \times \vec{a}_1)} \qquad \vec{b}_3 = \frac{2\pi\,\vec{a}_1 \times \vec{a}_2}{\vec{a}_3 \cdot (\vec{a}_1 \times \vec{a}_2)}$$

Note that $\vec{a}_i \cdot \vec{b}_j = 2\pi\delta_{ij}$

For cubic lattice $\left\{ \begin{array}{l} \vec{a}_i = a\,\hat{e}_i \\ \vec{b}_i = \dfrac{2\pi}{a}\hat{e}_i \end{array} \right.$