Day 16

→ Crystal structure descriptions :

— Lattice + motif (Atoms / molecules)
— Close packed / Interstitials

↓

Eutactic structures (almost close packed)

→ Perfect crystal

- Impossible
- Useless

Diffraction techniques

↓

X-Ray Diffraction (Chapter 11 from de Graef's book)

part of EM spectrum between UV and γ-rays

Scatters

→ In most crystals atoms are spaced several angstroms apart (Reason for choosing X-rays)

→ We try to use coherent and monochromatic radiation.

→ K: wave number (inverse length)
↳ in 3D, called as a wave vector ($\vec{k}$)

Natural coordinate system: Reciprocal space

→ If $\vec{r}$: real space —

$$\vec{r} = x_i \vec{a_i}$$
$$\vec{K} = k_i \vec{a_i}^*$$

Then $\vec{K} \cdot \vec{r} = k_i x_i$

$k_1, k_2, k_3 \rightarrow$ components of the wave vector along reciprocal space basis vectors.

Now, $E(\vec{r}, t) = A e^{2\pi i (\vec{K} \cdot \vec{r})}$

↳ temporal variation ignored

If $\vec{K} \cdot \vec{r} = 0$, then

$E(\vec{r}, t) = A$ (constant in a plane)

→ Phase difference ∝ path length difference

$$\boxed{\phi = \frac{2\pi}{\lambda} \Delta x}$$

In case of x-ray diffraction:

$$\boxed{\Delta x = 2d \sin\theta}$$

In case of constructive interference,

$$\boxed{2d \sin\theta = n\lambda}$$ (Bragg's law)

↓ william Lawrence Bragg

↓ order of diffraction (integers)

We may write,

$$2\left(\frac{d}{n}\right)\sin\theta = \lambda$$

What is d/n?

Let $(h\ k\ l)$ have interplanar spacing d_{hkl}

Same for $(nh\ nk\ nl) \rightarrow \frac{d_{hkl}}{n}$

↓ & very 'different' from $(h\ k\ l)$!

So we write

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

→ Problem:

Bcc iron

a.) Interplanar spacing for (2 2 0) plane set?
b.) Diffraction angle 2θ?

$a = 0.2866$ nm. Assume $\lambda = 0.179$ nm monochromatic radiation used.

(Ans.) a.) $$d = \frac{a}{\sqrt{h^2+k^2+l^2}} = \frac{0.2866}{2\sqrt{2}}\ \text{nm}$$

b.) $$2\theta = 2\sin^{-1}\frac{\lambda}{2d} = 2\sin^{-1}\frac{0.179\times 2\sqrt{2}}{2\times 0.2866}$$