We were analyzing the X-Ray Diffraction Pattern. and side tracked with the Reciprocal lattice.

There Let's go back to the X Ray Diffractions.

The quantity we have looked at to find the scattering amplitude:

$$A \cdot \int_{cell} dV\, n(r) \exp^{-iG.r} = S_G \rightarrow \underline{\text{structure factor.}}$$

$n(r) \longrightarrow$ is the electron density

If we write $n_j \rightarrow$ the electron density associated with the j^{th} atom.

$$n(r) = \sum_{j=1}^{s} n_j(r - r_j)$$ s = the number of atoms in the basis

$$S_G = \int_{cell} dV\, n(r) \exp^{-iG.r}$$

$$= \sum_j \int dV\, n_j(r - r_j) \exp^{-iG.r}$$

$$= \sum_j \exp^{-iG.r_j} \underbrace{\int dV\, n_j(\rho)\, e^{-iG.\rho}}_{f_j} \qquad \rho = r - r_j$$

$$S_j = \sum_j \exp^{-iG.r_j} f_j$$ f_j is an atomic factor

$$r_j = x_j \bar{a} + y_j \bar{b} + z_j \bar{c}$$

$$G = h \bar{A} + k \bar{B} + l \bar{C}$$

$$S_{hkl} = \sum_j f_j \exp^{-i[2\pi (x_j h + y_j k + z_j l)}$$

S_{hkl} ↑ Structure Factor

x_j , y_j , z_j ⟶ Atomic Positions

BCC We consider BCC lattice as a cube Lattice with a basis.

$(x_j , y_j , z_j) \longrightarrow (0, 0, 0) \left(\frac{1}{2} , \frac{1}{2} , \frac{1}{2}\right)$

$$S_{hkl} = f\left[1 + \exp^{-i\pi[h+k+l]}\right]$$

$S_{hkl} \longrightarrow 0$ { If $h+k+l$ = odd integer }

$\longrightarrow 2f$ { If $h+k+l$ = even integer }

For example, Metallic Sodium has a BCC structure. The Diffraction spectrum does not contain lines such as (1 0 0) (3 0 0) (1 1 1) (9 2 1). But lines such as (2 0 0) (1

In the similar way, we can find that for a

Fcc crystal

$$S_{hkl} = f\left[1 + e^{-i\pi(k+l)} + e^{-i\pi(h+l)} + e^{-i\pi(h+k)}\right]$$

$= 4f$ ← If h, k, l all odd or all even

$= 0$ ← If h, k, l mixed parity.

Let's say we get the Bragg Reflection for a cubic crystal. In order to identify if the peaks are SC/Fcc/BCC we need to analyse the peaks and find out all the possible $h^2 + k^2 + l^2$ values.

$h^2 + k^2 + l^2$	⟶	
	1	(1 0 0)
	2	(1 1 0)
	3	(1 1 1)
	4	(2 0 0)
	5	(2 0 1)
	6	(2 1 1)
	~~7~~	
	8	(2 2 0)
	9	(3 0 0) (3 2 1)
	10	(3 1 0)

hkl	$h^2+k^2+l^2$	SC	BCC	FCC
(100)	1	✓	X	X
(110)	2	✓	✓	X
(111)	3	✓	X	✓
(200)	4	✓	✓	✓
(210)	5	✓	X	X
(211)	6	✓	✓	X
?	7	No	No	No
(220)	8	✓	✓	✓
(300) (221)	9	✓	X	X
(310)	10	✓	✓	X
(311)	11	✓	X	✓

Let's Look at some examples :

We use a monochromatic X-Ray with $\lambda = 1.5418$ for X-Ray diffraction to identify a crystal (which is known to be mono atomic and belong to the cubic system). Diffraction peaks are reported at $2\theta = 44.48, 51.83, 76.35, 92.90$ $98.40, 121.87$ ..... Find the Bravais Lattice type and the Crystal cell size a.

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

$$\frac{2a}{\sqrt{h^2+k^2+l^2}} \sin\theta = \lambda \qquad n = 1$$

$$\frac{4a^2}{(h^2+k^2+l^2)} \sin^2\theta = \lambda^2$$

$$\frac{4a^2}{\lambda^2} = \frac{\sin^2\theta}{h^2+k^2+l^2}$$

We first calculal $\sin^2\theta$

2θ	θ	$\sin^2\theta$	$\sin^2\theta / \sin^2\theta_1$ (normalizing)
44.48	22.24	0.143252	1.00 → 1.00 → 3
51.83	25.915	0.191002	1.3333 → $\frac{4}{3}$ → 4
76.35	38.175	~~0.382005~~ 0.382005	2.6666 → $\frac{8}{3}$ → 8
92.90	46.45	0.525296	3.66694 → $\frac{11}{3}$ → 11
98.40	49.2	0.573043	4.000 → $\frac{12}{3}$ → 12
121.87	60.935	0.763997	5.33334 → $\frac{16}{3}$ → 16

We identify that $\sin^2\theta$ has a pattern

3 , 4 , 8 , 11 , 12

In other words :

$$\frac{\sin^2\theta}{h^2+k^2+l^2} = \text{Constant}$$ if we choose $h^2+k^2+l^2 \longrightarrow$ 3, 4, 8, 11,

⇒ By looking at the previous table

This is a FCC system.

Now $$\frac{4a^2}{\lambda^2} = \frac{\sin^2\theta}{h^2+k^2+l^2}$$

Let's consider the first peak $\theta = 22.24$

$\sin^2\theta = 0.143252$

$h^2+k^2+l^2 = 3$

$$\frac{4a^2}{\lambda^2} = \frac{0.143252}{3}$$

$$a^2 = \frac{0.143252}{3\times 4} \times (1.5418)^2 \text{ °A}^2 = 0.0983$$

$a = 0.1684$ °A

$a = 1.684$ nm

Surfaces and Interfaces

Introduction :

What happens when a surface of a crystal is open.

Geometry of Interfaces :

It can be a place where crystals comes an end.

or one crystal meets another crystal.

What happens when a crystal is sliced in a plane.

~~The way in which it fails has to do with~~

Crystals deforms as it approches boundary.

=▷ It may involve the formation of an entirely new crystal structure right at the interface

=▷ Surface Reconstruction

Surface Reconstruction

Coherent & Commensurate Interfaces

When two crystals meet, the main question is if they will mesh well.

If two crystals meet, if all the atoms are in perfect regis with one another

$\Rightarrow$ It is a ~~Coherent Surface~~ Coherent Interface.

$\Rightarrow$ That process of growth is called

EPITAXY

Commensurate Interface.

Two surfaces are commensurate if there i some larger two dimensional lattice on which they coincide

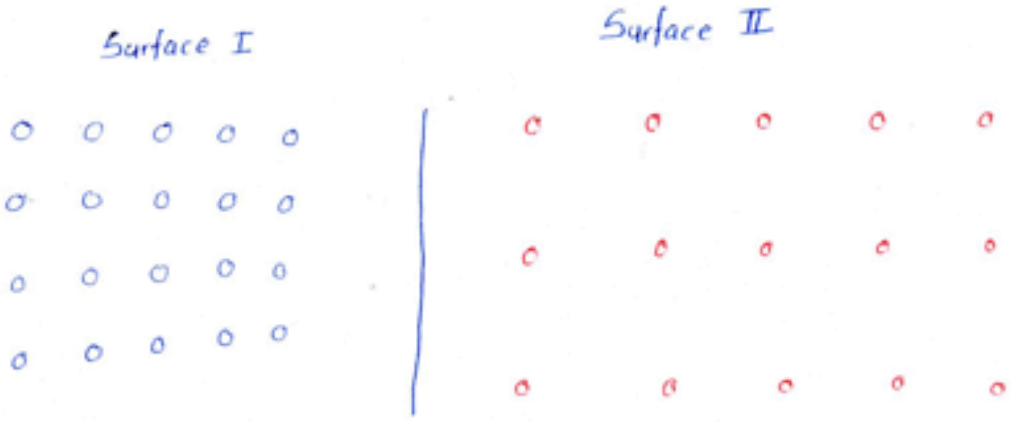
$\bar{a}_1, \bar{a}_2 \longrightarrow$ primitive vectors of the surface 1

$\bar{b}_1, \bar{b}_2 \longrightarrow$ primitive vector of the surface 2

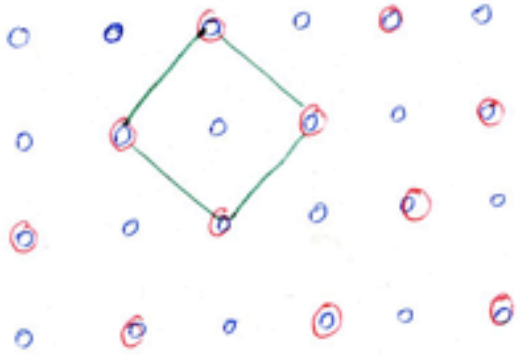
Then the two surfaces are commensurate if there is an infinite set of integers

$$n_1 \bar{a}_1 + n_2 \bar{a}_2 = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} (m_1 \bar{b}_1 + m_2 \bar{b}_2)$$

Now this larger cell is called a SUPERCELL



We can Find a commensurate configuration for the surface I & surface II as follows.



Now the Green color cell is a commensurate cell for both the surface I & surface II.