

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:

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

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

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

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

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

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

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

$$S_G = \sum_j \exp^{-iG \cdot r_j} f_j \quad f_j \text{ is an atomic factor}$$

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

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

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

↑  
Structure Factor

$x_j, y_j, z_j \longrightarrow$  Atomic Positions

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

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

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

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

$$\longrightarrow 2f \quad \left\{ \text{If } h+k+l = \text{even integer} \right\}$$

For example, Metallic Sodium has a BCC structure. The Diffraction spectrum does not contain lines such as (100) (300) (111) (221). But lines such as (200) (400) (211) (220) (311) (420) (440) (404) (444) (600) (660) (666) (800) (880) (888) (110) (200) (210) (220) (310) (320) (330) (410) (420) (430) (440) (510) (520) (530) (540) (610) (620) (630) (640) (650) (660) (700) (770) (777) (800) (880) (888) (900) (990) (999) (112) (202) (212) (222) (312) (322) (332) (412) (422) (432) (442) (512) (522) (532) (542) (612) (622) (632) (642) (652) (662) (702) (772) (777) (802) (882) (888) (902) (992) (999) (114) (204) (214) (224) (314) (324) (334) (414) (424) (434) (444) (514) (524) (534) (544) (614) (624) (634) (644) (654) (664) (704) (774) (777) (804) (884) (888) (904) (994) (999) (116) (206) (216) (226) (316) (326) (336) (416) (426) (436) (446) (516) (526) (536) (546) (616) (626) (636) (646) (656) (666) (706) (776) (777) (806) (886) (888) (906) (996) (999) (118) (208) (218) (228) (318) (328) (338) (418) (428) (438) (448) (518) (528) (538) (548) (618) (628) (638) (648) (658) (668) (708) (778) (777) (808) (888) (888) (908) (998) (999) (120) (210) (220) (320) (330) (420) (430) (440) (520) (530) (540) (620) (630) (640) (650) (660) (720) (730) (740) (750) (760) (770) (780) (790) (820) (830) (840) (850) (860) (870) (880) (890) (920) (930) (940) (950) (960) (970) (980) (990) (122) (222) (322) (422) (522) (622) (722) (822) (922) (124) (224) (324) (424) (524) (624) (724) (824) (924) (126) (226) (326) (426) (526) (626) (726) (826) (926) (128) (228) (328) (428) (528) (628) (728) (828) (928) (130) (230) (330) (430) (530) (630) (730) (830) (930) (132) (232) (332) (432) (532) (632) (732) (832) (932) (134) (234) (334) (434) (534) (634) (734) (834) (934) (136) (236) (336) (436) (536) (636) (736) (836) (936) (138) (238) (338) (438) (538) (638) (738) (838) (938) (140) (240) (340) (440) (540) (640) (740) (840) (940) (142) (242) (342) (442) (542) (642) (742) (842) (942) (144) (244) (344) (444) (544) (644) (744) (844) (944) (146) (246) (346) (446) (546) (646) (746) (846) (946) (148) (248) (348) (448) (548) (648) (748) (848) (948) (150) (250) (350) (450) (550) (650) (750) (850) (950) (152) (252) (352) (452) (552) (652) (752) (852) (952) (154) (254) (354) (454) (554) (654) (754) (854) (954) (156) (256) (356) (456) (556) (656) (756) (856) (956) (158) (258) (358) (458) (558) (658) (758) (858) (958) (160) (260) (360) (460) (560) (660) (760) (860) (960) (162) (262) (362) (462) (562) (662) (762) (862) (962) (164) (264) (364) (464) (564) (664) (764) (864) (964) (166) (266) (366) (466) (566) (666) (766) (866) (966) (168) (268) (368) (468) (568) (668) (768) (868) (968) (170) (270) (370) (470) (570) (670) (770) (870) (970) (172) (272) (372) (472) (572) (672) (772) (872) (972) (174) (274) (374) (474) (574) (674) (774) (874) (974) (176) (276) (376) (476) (576) (676) (776) (876) (976) (178) (278) (378) (478) (578) (678) (778) (878) (978) (180) (280) (380) (480) (580) (680) (780) (880) (980) (182) (282) (382) (482) (582) (682) (782) (882) (982) (184) (284) (384) (484) (584) (684) (784) (884) (984) (186) (286) (386) (486) (586) (686) (786) (886) (986) (188) (288) (388) (488) (588) (688) (788) (888) (988) (190) (290) (390) (490) (590) (690) (790) (890) (990) (192) (292) (392) (492) (592) (692) (792) (892) (992) (194) (294) (394) (494) (594) (694) (794) (894) (994) (196) (296) (396) (496) (596) (696) (796) (896) (996) (198) (298) (398) (498) (598) (698) (798) (898) (998) (200) (300) (400) (500) (600) (700) (800) (900) (1000)

In the similar way, we can find that for a

FCC crystal

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

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

$= 0 \leftarrow$  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 analyze the peaks and find out all the possible  $h^2 + k^2 + l^2$  values.

$h^2 + k^2 + l^2 \rightarrow$	1	(100)
	2	(110)
	3	(111)
	4	(200)
	5	(201)
	6	(211)
	<del>7</del>	
	8	(220)
	9	(300) (221)
	10	(310)

$hkl$	$h^2 + k^2 + l^2$	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	☹
(220)	8	✓	✓	✓
(300) (221)	9	✓	X	X
(310)	10	✓	✓	X
(311)	11	✓	X	✓

Let's Look at some examples :

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

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

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

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

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

We first calculate  $\sin^2 \theta$

$2\theta$	$\theta$	$\sin^2 \theta$	$\sin^2 \theta / \sin^2 \theta_1$ (normalizing)
44.48	22.24	0.143252	1.00 $\rightarrow$ 1.00 $\rightarrow$ 3
51.83	25.915	0.191002	1.3333 $\rightarrow$ $\frac{4}{3}$ $\rightarrow$ 4
76.35	38.175	<del>0.382005</del> 0.382005	2.6666 $\rightarrow$ $\frac{8}{3}$ $\rightarrow$ 8
92.90	46.45	0.525296	3.66694 $\rightarrow$ $\frac{11}{3}$ $\rightarrow$ 11
98.40	49.2	0.573049	4.000 $\rightarrow$ $\frac{12}{3}$ $\rightarrow$ 12
121.87	60.935	0.763997	5.3334 $\rightarrow$ $\frac{16}{3}$ $\rightarrow$ 16

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

3, 4, 8, 11, 12

In other words:

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

$\Rightarrow$  By looking at the previous table

This is a FCC system.

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

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

$$\sin^2 \theta = 0.143252$$

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

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

$$a^2 = \frac{0.143252}{3 \times 4} \times (1.5418)^2 \text{ \AA}^2 = 0.0283$$

$$a = 0.1684 \text{ \AA}$$

$$a = 1.684 \text{ nm}$$

## Surfaces and Interfaces

### Introduction :

What happens when a surface of a crystal is open.

### Geometry of Interfaces :

It can be a place where crystal~~s~~ 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~~is~~ as it approaches boundary.

⇒ It may involve the formation of an entirely new crystal structure right at the interface.

⇒ Surface Reconstruction

### Surface Reconstruction

## Coherent & Commensurate

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

If two crystals meet, if all the atoms are in perfect register 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 is some larger two dimensional lattice on which they coincide

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

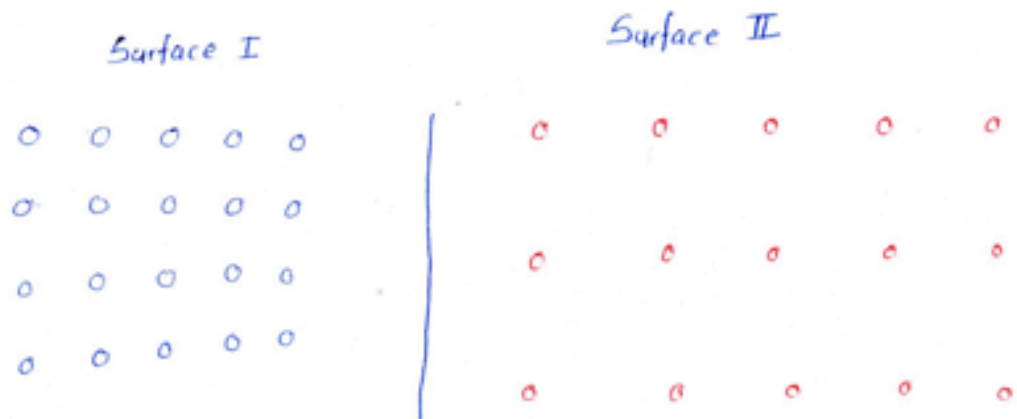
$\bar{b}_1, \bar{b}_2 \rightarrow$  primitive vector of the surface 2

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

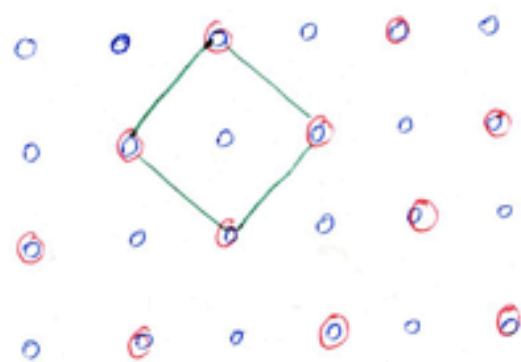
$$n_1 \bar{a}_1 + n_2 \bar{a}_2 = \begin{pmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{pmatrix} (m_1 \bar{b}_1 + m_2 \bar{b}_2)$$

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.