Phys 425
Lecture 5

Last time

Laue condition

$\vec{K}' - \vec{K} = \vec{G}$ "physical picture"

Bragg scattering

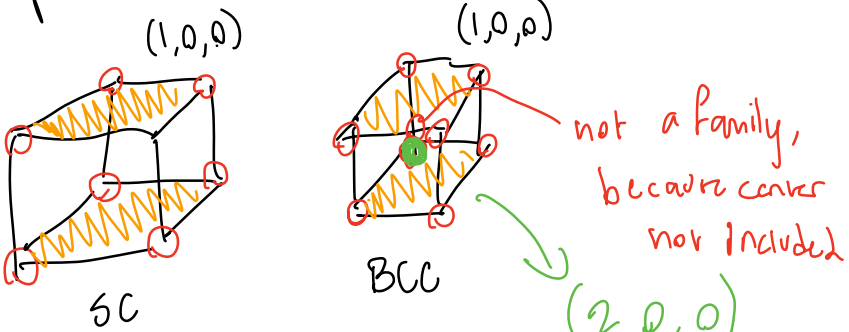
$2 d_{hkl} \sin\theta = n\lambda$ "practical picture"

$\hookrightarrow d_{hkl} = \frac{\lambda}{2\sin\theta} = \frac{a}{\sqrt{h^2+k^2+l^2}}$

Selection Rules

You can pick any set of (h,k,l) but there's no guarantee that it will be a family of lattice planes.

eg

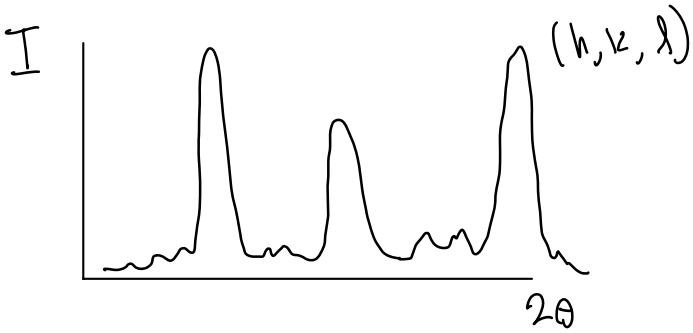


SC

This means $(1,0,0)$ would show up as a peak in the diffraction pattern for simple cubic. Not for the BCC.

→ powder diffraction pattern

(SC)



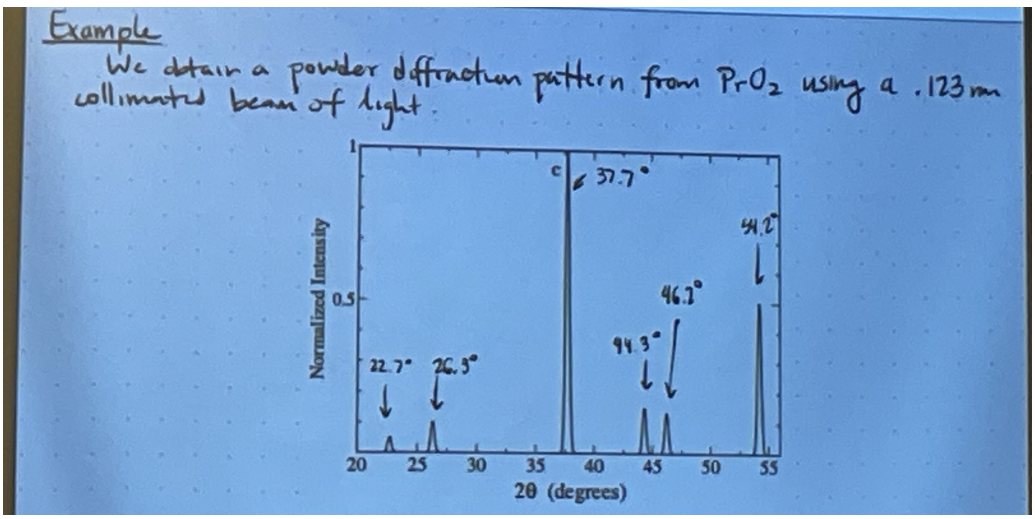
Conceptually: missing peaks would occur due to two sets of (1,0,0) planes destructively interfering.

Selection Rules:

Lattice	(h,k,l)
SC	any (h,k,l) allowed
BCC	h+k+l must be even
FCC	h,k,l all odd or all even.

Example

We obtain a powder diffraction pattern from PrO_2 using a .123 nm collimated beam of light.



We need to find some # such that $\# \times \frac{1}{d^2} \rightarrow$ integer

↳ easiest method

find

$\frac{d^2_{max}}{d^2} \rightarrow \frac{nd^2_{max}}{d^2}$ ← integer

2θ	$d_{hkl} = \frac{\lambda}{2\sin\theta}$	$\frac{d^2_{max}}{d^2}$	$\frac{3d^2_{max}}{d^2}$	(h,k,l)	$a = d\sqrt{h^2+k^2+l^2}$
22.7°	0.313 nm	1	3	(1,1,1)	.542 nm
26.3°	0.27 nm	1.33	3.99	(2,0,0)	.540 nm
37.7°	0.19 nm	2.69	8.07	(2,2,0)	.537 nm
44.3°	0.163 nm	3.67	11.01	(3,1,1)	.541 nm
46.2°	0.157 nm	3.97	11.91	(2,2,2)	.544 nm
54.2°	0.135 nm	5.35	16.05	(4,0,0)	.540 nm

notice all ≈ divided by 3

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

$a \approx .541$ nm

We know the (h,k,l)'s corresponding to the peaks.

↓

Compare to selection rules
to determine the lattice structure.

↓

FCC Lattice.

Microscopic Properties of Bonding (Friday's lecture = Covalent bonding)

Generally, a bond consists of two things

- something that attracts the two atoms together
  - attractive force
- something that keeps the atoms apart
  - repulsive force

We write this as

$$\phi(r) = \underbrace{\frac{A}{r^n}}_{\text{repulsive force}} - \underbrace{\frac{B}{r^m}}_{\text{attractive force.}}$$

$r \rightarrow$ atomic distance

$\phi \rightarrow$ potential

$A, B \rightarrow$ constants

$n, m \rightarrow$ integers

We must have

$m < n$

↳ from this

Repulsion has to dominate at small distances.