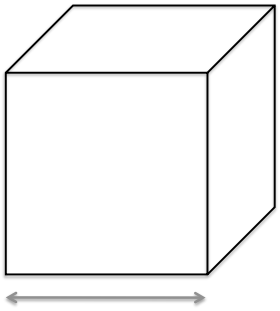
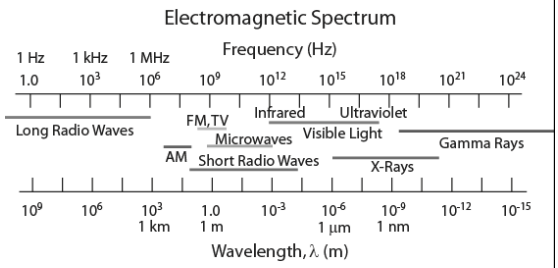
Let's start with a simple cubic structure…

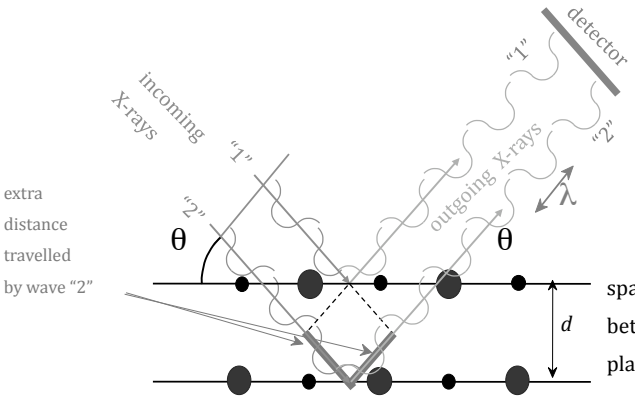
$a = 2R \sim 2\,(0.1\text{nm}) = 0.2\text{ nm} \sim \lambda$





X-rays!!!!

When do we get constructive interference?

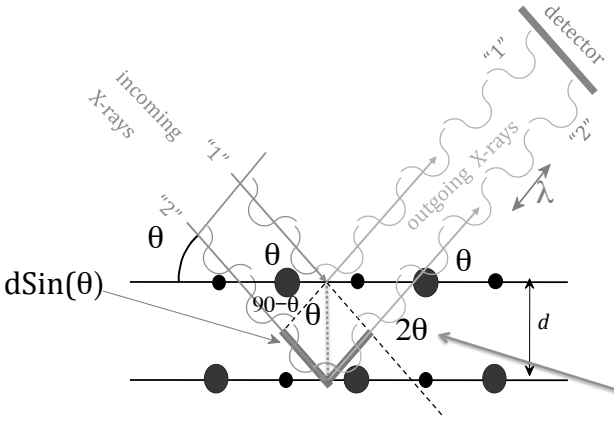


extra distance travelled by wave "2"

reflections must be in phase for a detectable signal

Adapted from Fig. 3.19, *Callister 7e.*

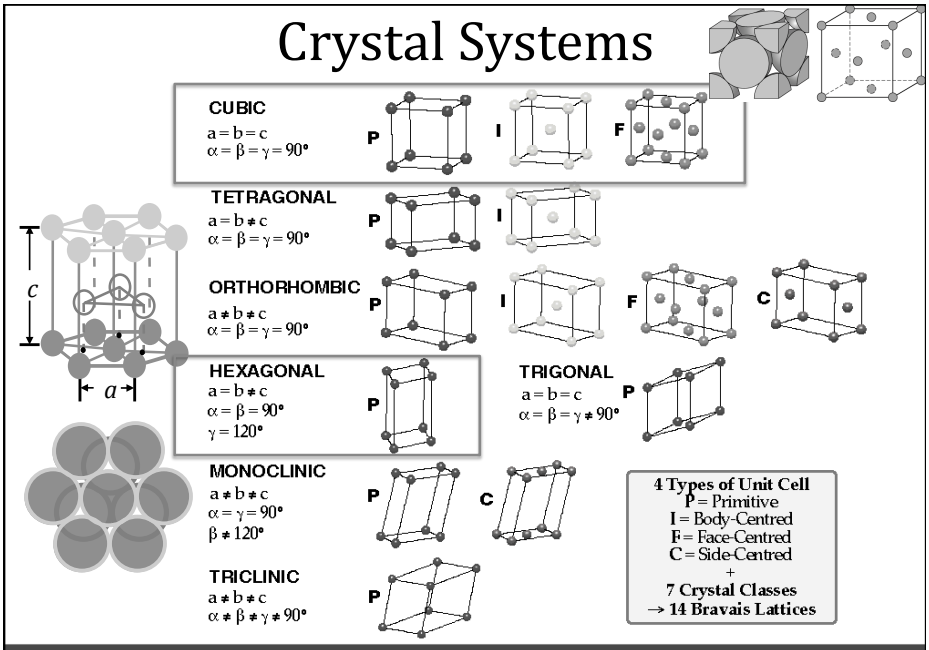
$\Delta L = n\lambda = 2d\sin(\theta)$ Bragg's law



Adapted from Fig. 3.19, *Callister 7e.*

We will plot 2θ vs. intensity

Crystal Systems



Unit cell:

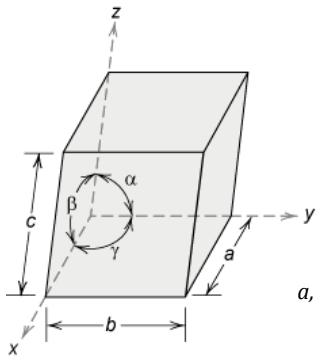
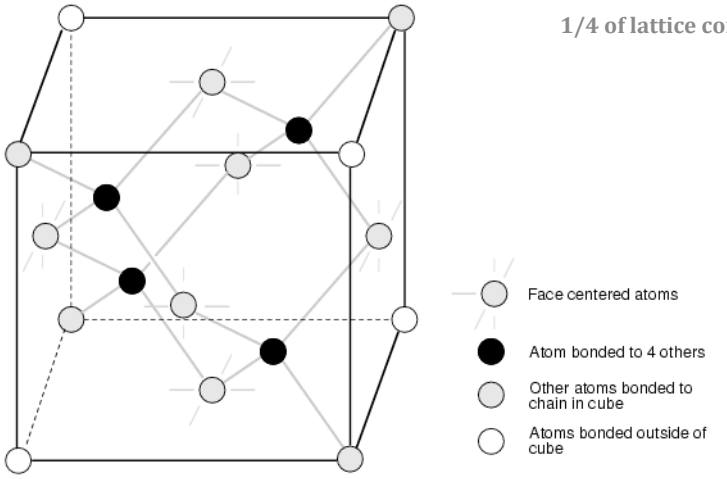


Fig. 3.4, *Callister 7e.*

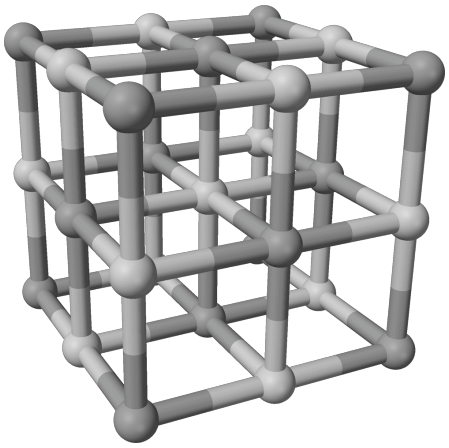
a, *b*, and *c* are the lattice constants

Diamond: FCC structure with two atom base (0,0,0), (1/4, 1/4, 1/4)

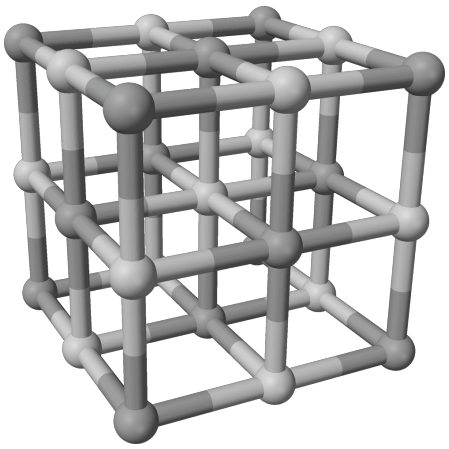
1/4 of lattice constant !!



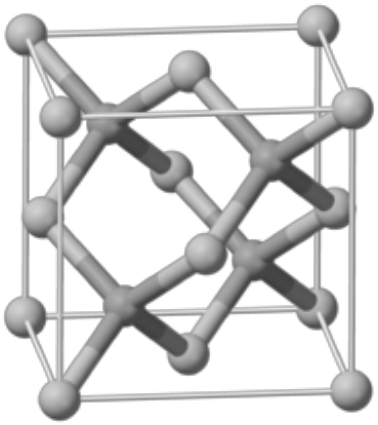
What is the crystal structure / base of NaCl?



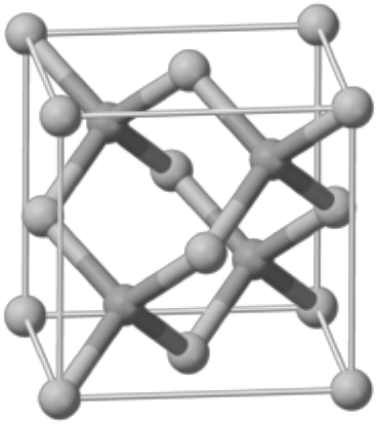
FCC with 2 atom base: (0,0,0), (1/2, 1/2, 1/2)

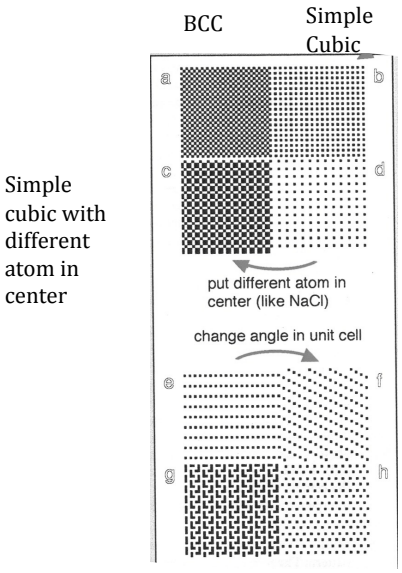


What is the crystal structure / base of ZnSe?



Like diamond: FCC structure with two atom base (0,0,0), (1/4, 1/4, 1/4)



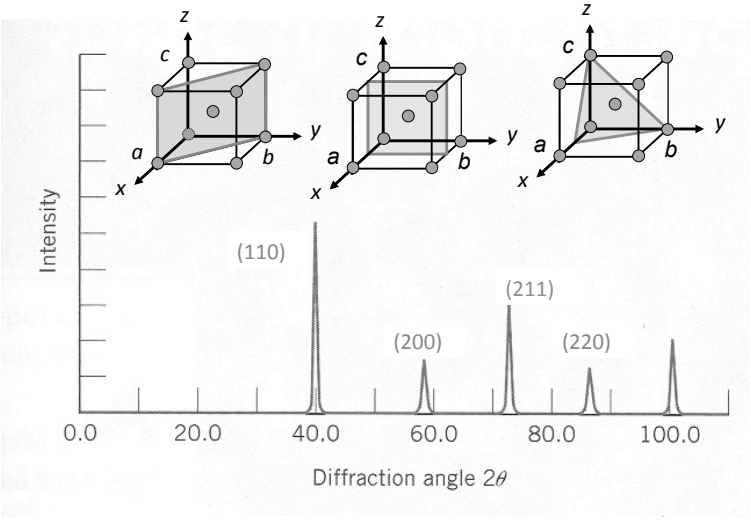


Simple cubic with different atom in center

Simple Cubic with larger d spacing

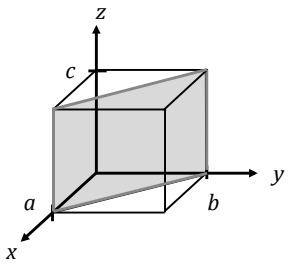
Hexagonal cell

Example: X-ray diffraction of Tungsten

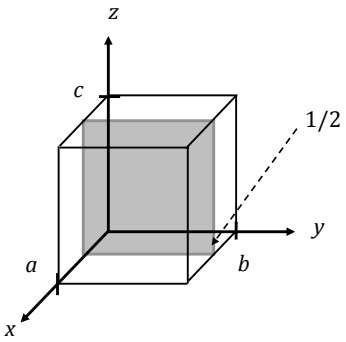


Crystallographic Planes

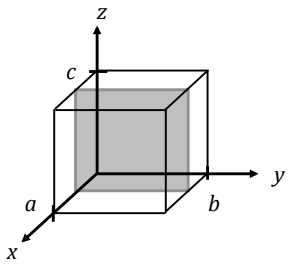
example		*a*	*b*	*c*
1.	Intercepts	1	1	∞
2.	Reciprocals	1/1	1/1	1/∞
		1	1	0
3.	Reduction	1	1	0
4.	Miller Indices	(110)		



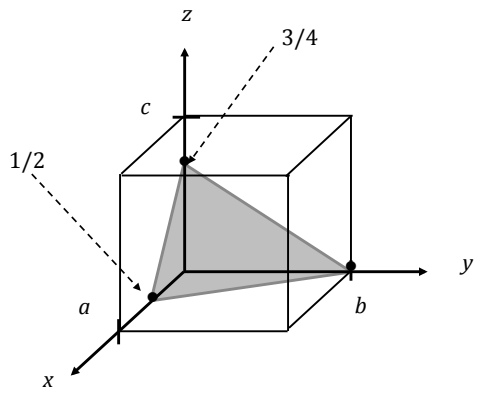
What are the Miller indices?



example	*a*	*b*	*c*
1. Intercepts	1/2	∞	∞
2. Reciprocals	2	1/∞	1/∞
	2	0	0
3. Reduction	2	0	0
4. Miller Indices	(200)		



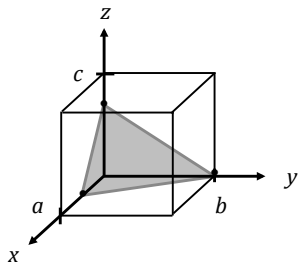
What are the Miller indeces?



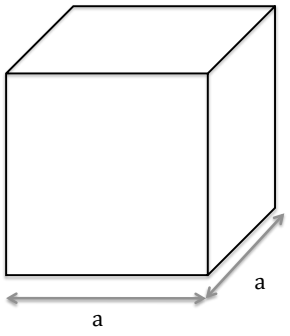
Crystallographic Planes

example	*a*	*b*	*c*
1. Intercepts	1/2	1	3/4
2. Reciprocals	2	1	4/3
3. Reduction	6	3	4

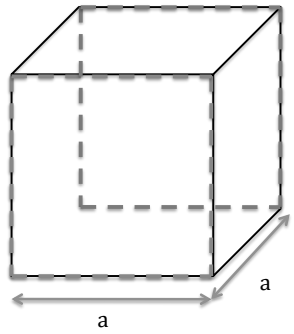
4. Miller Indices (634)



What is the interplanar spacing d for {100}?



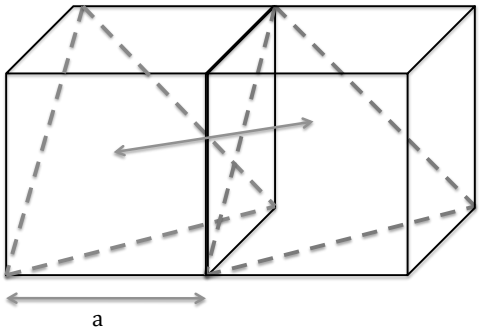
What is the interplanar spacing d?



{hkl} = {100}

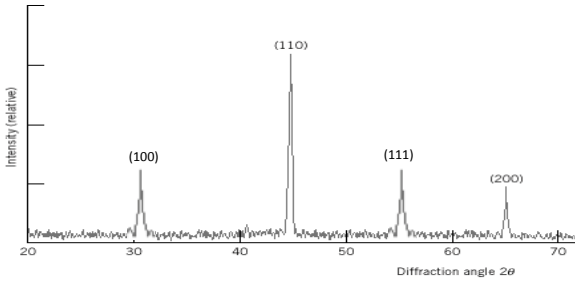
d = a

What is the interplanar spacing d for {111}?



{hkl} = {111} d = a/√(3)

Simple cubic:



Why is (100) peak missing?

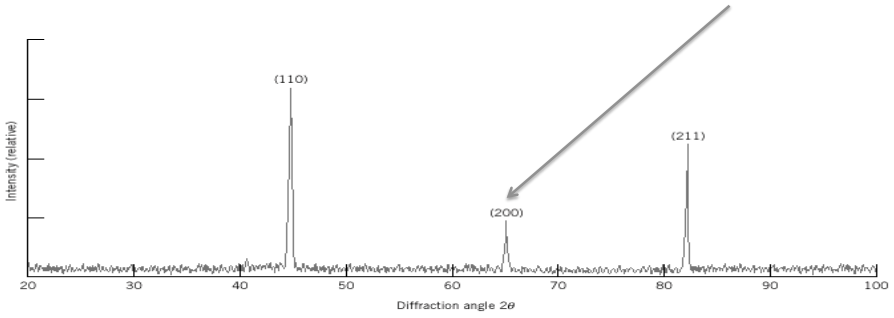
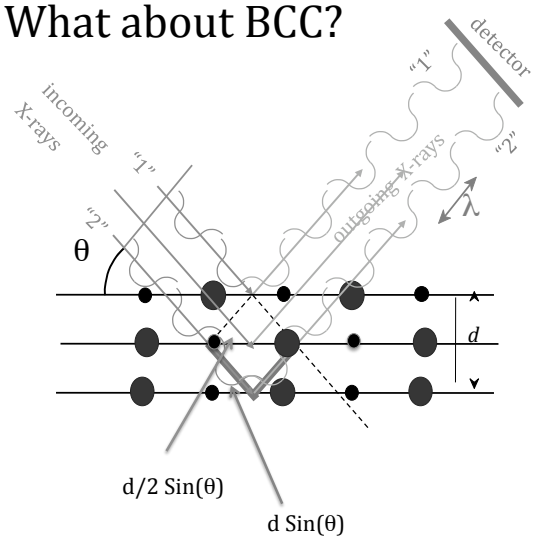


FIGURE 3.20 Diffraction pattern for polycrystalline α-iron.

What about BCC?



If $d \sin(\theta) = n\lambda$
then $d/2 \sin(\theta) = n\lambda / 2$

Destructive interference!!!

All of the odd-number diffractions (h+k+l = odd) are gone.

Bragg diffraction for cubic structures

$\Delta L = n\lambda = 2d\sin(\theta)$ Bragg's law

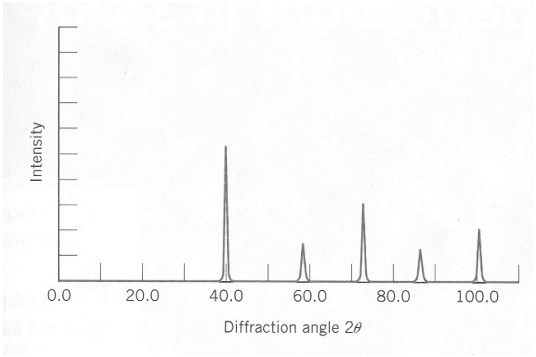
$d_{hkl} = a/\sqrt{(h^2 + k^2 + l^2)}$

Type	Rules
Simple cubic	all (hkl)
BCC	h + k + l = even
FCC	h, k, l all odd or all even

Example: X-ray diffraction of Tungsten

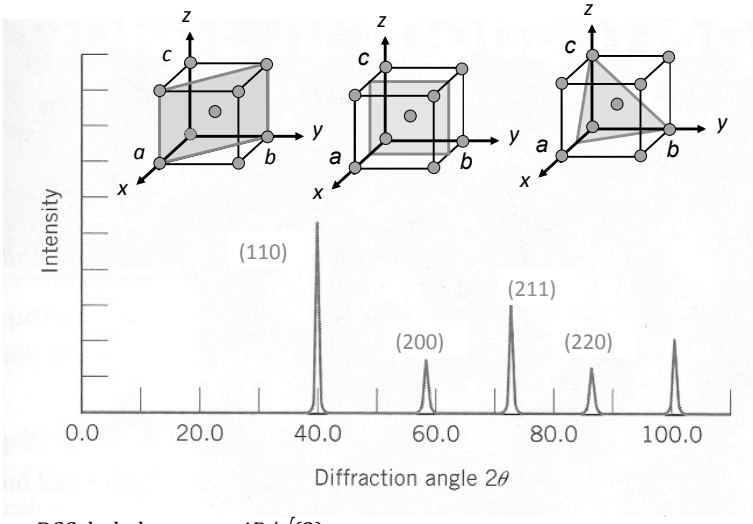
λ = 0.1542nm, BCC tungsten, R=0.137nm

Index each of the peaks



BCC: h+k+l even, a = 4R/√(3)

Example: X-ray diffraction of Tungsten



BCC: h+k+l even, a = 4R/√(3)