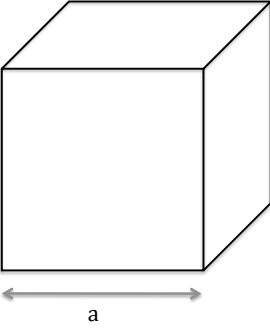
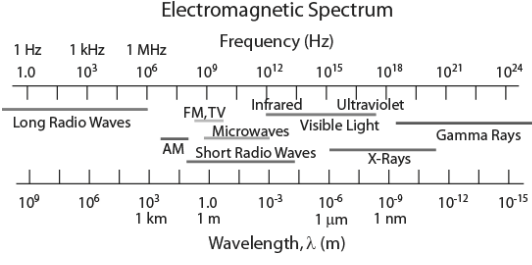


Let's start with a simple cubic structure...

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



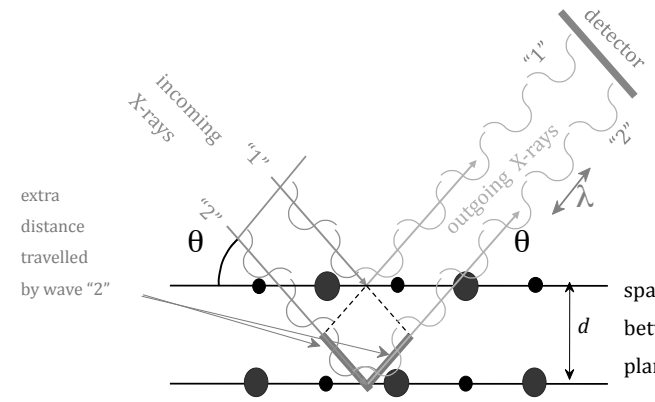
Electromagnetic Spectrum



X-rays!!!!

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When do we get constructive interference?



incoming "1"

outgoing X-rays "1" "2"

detector

spacing between planes d

θ

λ

extra distance travelled by wave "2"

reflections must be in phase for a detectable signal

Adapted from Fig. 3.19, Callister 7e.

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

incoming "1" "2" X-rays
outgoing X-rays "1" "2"
detector
 λ
 d
 2θ
 θ
 θ
 $90-\theta$
 $d\sin(\theta)$

Adapted from Fig. 3.19, Callister 7e.

We will plot 2θ vs. intensity

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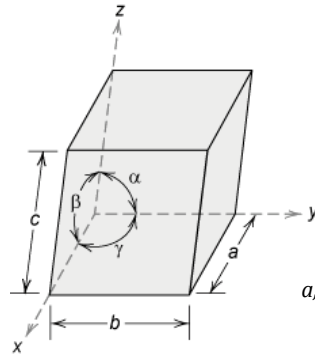
Crystal Systems

| | | | |
|---|------------------|--|------------------|
| <p>CUBIC $a = b = c$ $\alpha = \beta = \gamma = 90^\circ$</p> | <p>P </p> | <p>I </p> | <p>F </p> |
| <p>TETRAGONAL $a = b \neq c$ $\alpha = \beta = \gamma = 90^\circ$</p> | <p>P </p> | <p>I </p> | |
| <p>ORTHORHOMBIC $a \neq b \neq c$ $\alpha = \beta = \gamma = 90^\circ$</p> | <p>P </p> | <p>I </p> | <p>F </p> |
| <p>HEXAGONAL $a = b \neq c$ $\alpha = \beta = 90^\circ$ $\gamma = 120^\circ$</p> | <p>P </p> | <p>TRIGONAL $a = b = c$ $\alpha = \beta = \gamma \neq 90^\circ$</p> | <p>P </p> |
| <p>MONOCLINIC $a \neq b \neq c$ $\alpha = \gamma = 90^\circ$ $\beta \neq 90^\circ$</p> | <p>P </p> | <p>C </p> | |
| <p>TRICLINIC $a \neq b \neq c$ $\alpha \neq \beta \neq \gamma \neq 90^\circ$</p> | <p>P </p> | | |

4 Types of Unit Cell
P = Primitive
I = Body-Centred
F = Face-Centred
C = Side-Centred
 +
7 Crystal Classes
 → **14 Bravais Lattices**

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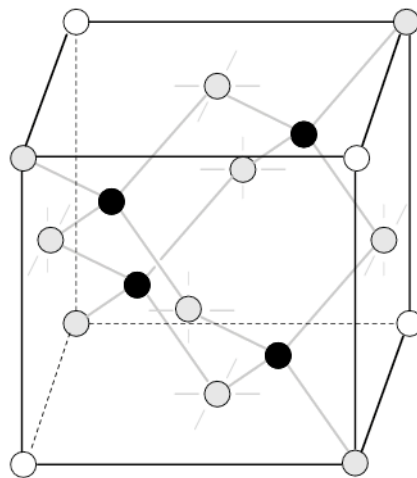
Unit cell:



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

Fig. 3.4, Callister 7e.

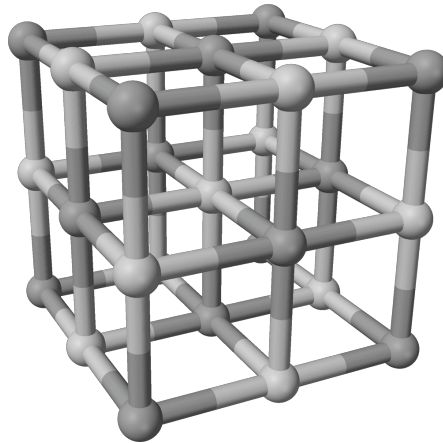
Diamond: FCC structure with two atom base $(0,0,0), (1/4, 1/4, 1/4)$



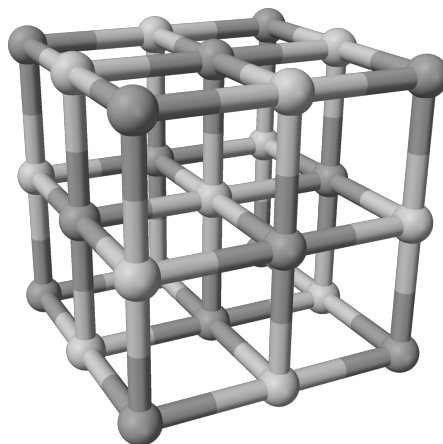
1/4 of lattice constant !!

- Face centered atoms
- Atom bonded to 4 others
- Other atoms bonded to chain in cube
- Atoms bonded outside of cube

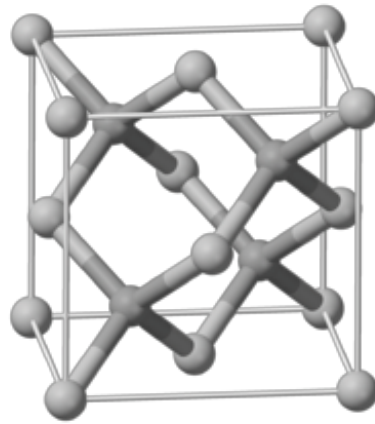
What is the crystal structure / base of NaCl?



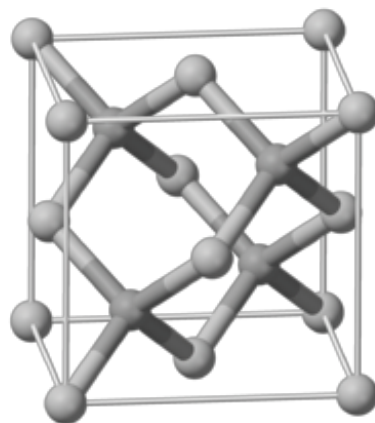
FCC with 2 atom base: $(0,0,0)$, $(1/2, 1/2, 1/2)$

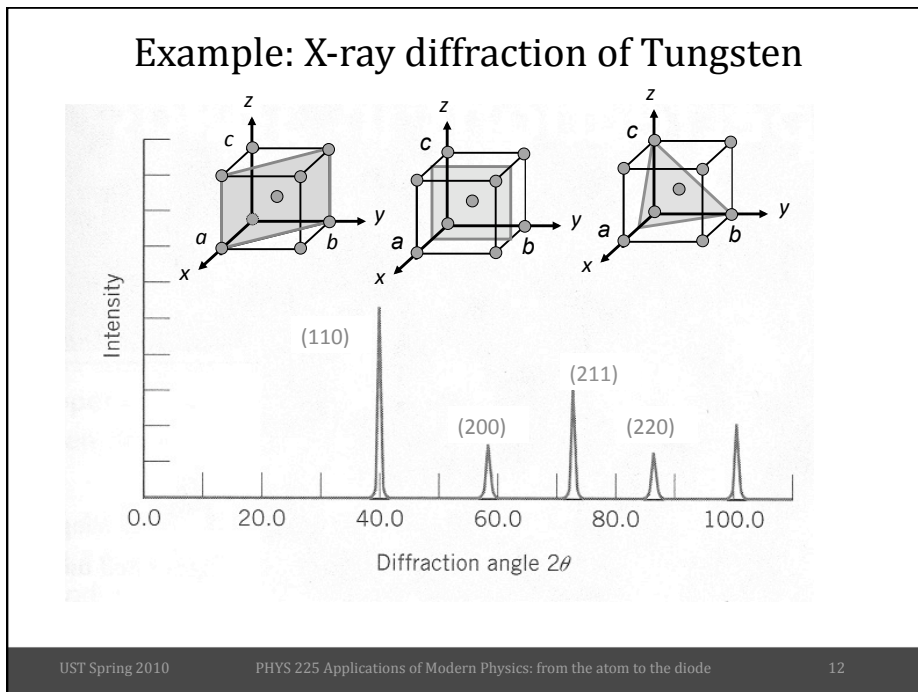
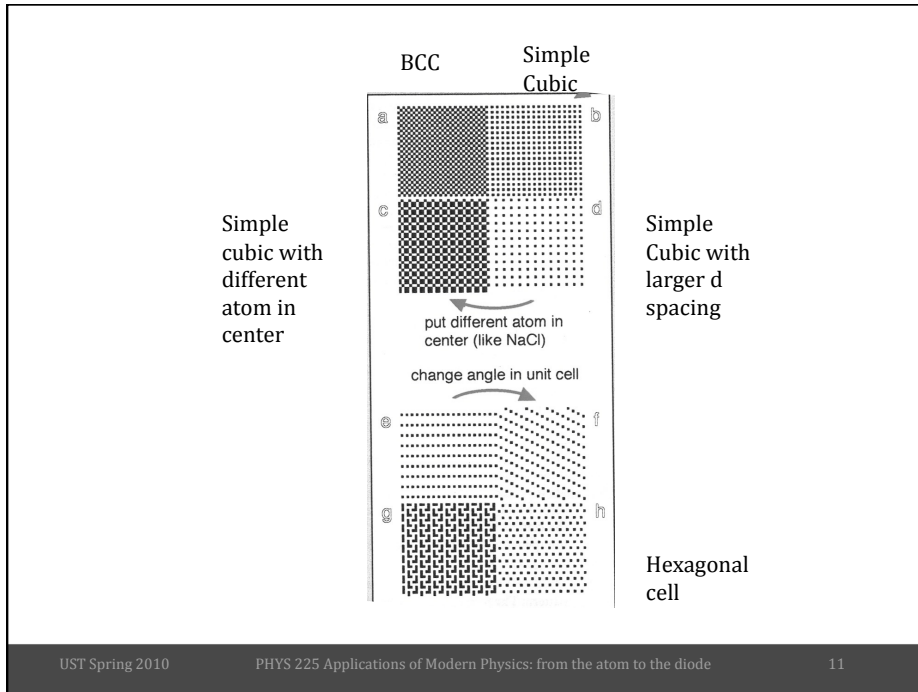


What is the crystal structure / base of ZnSe?



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

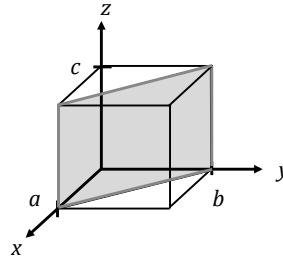




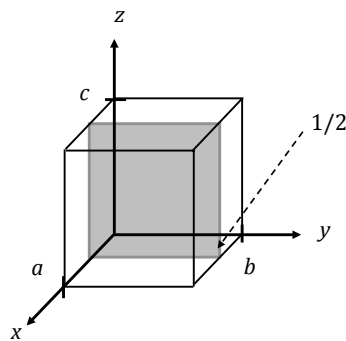
Crystallographic Planes

example

| | | | |
|-------------------|-------|-------|------------|
| 1. Intercepts | a | b | c |
| | 1 | 1 | ∞ |
| 2. Reciprocals | $1/1$ | $1/1$ | $1/\infty$ |
| | 1 | 1 | 0 |
| 3. Reduction | 1 | 1 | 0 |
| 4. Miller Indices | (110) | | |

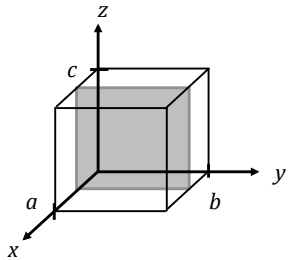


What are the Miller indices?



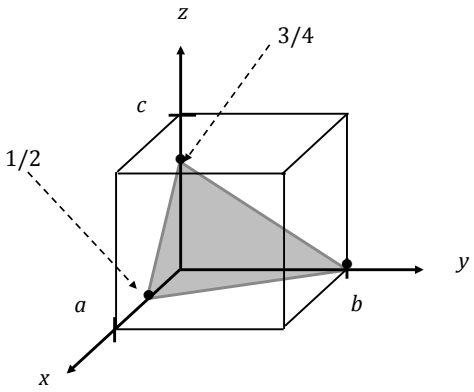
example

| | | | |
|-------------------|---------|------------|------------|
| | a | b | c |
| 1. Intercepts | $1/2$ | ∞ | ∞ |
| 2. Reciprocals | 2 | $1/\infty$ | $1/\infty$ |
| 3. Reduction | 2 | 0 | 0 |
| 4. Miller Indices | (200) | | |



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What are the Miller indices?



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Crystallographic Planes

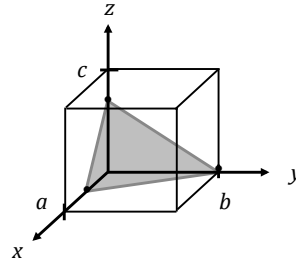
example

1. Intercepts
2. Reciprocals

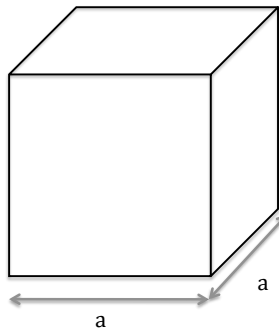
| a | b | c |
|-------|-----|-------|
| $1/2$ | 1 | $3/4$ |

3. Reduction
4. Miller Indices (634)

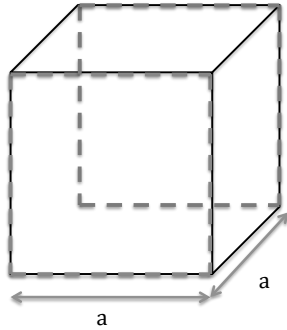
| | | |
|-----|-----|-------|
| 2 | 1 | $4/3$ |
| 6 | 3 | 4 |



What is the interplanar spacing d for $\{100\}$?



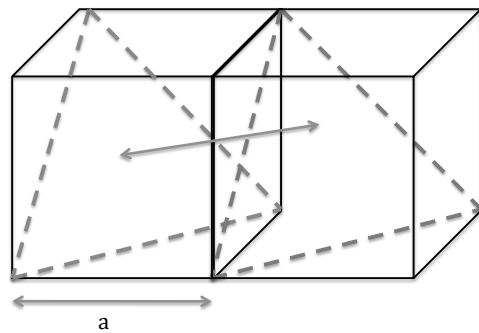
What is the interplanar spacing d ?



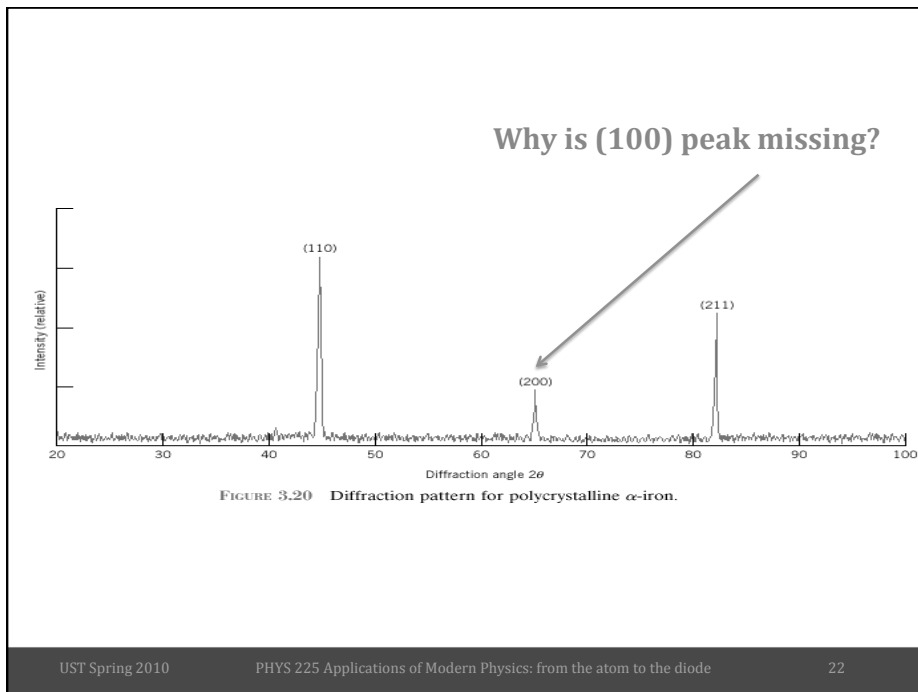
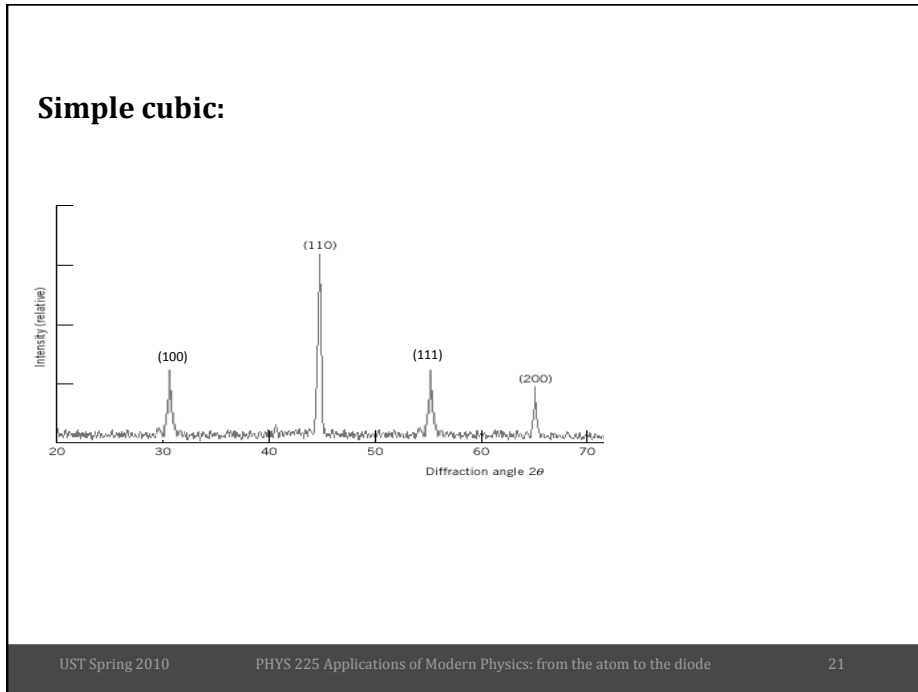
$$\{hkl\} = \{100\}$$

$$d = a$$

What is the interplanar spacing d for $\{111\}$?



$$\{hkl\} = \{111\} \quad d = a/\sqrt{3}$$



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 ($h+k+l = \text{odd}$)
are gone.

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Bragg diffraction for cubic structures

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

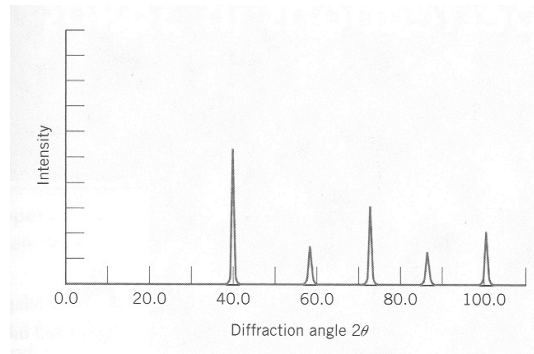
$$d_{hkl} = a/\sqrt{(h^2 + k^2 + l^2)}$$

| <u>Type</u> | <u>Rules</u> |
|--------------|-------------------------------|
| Simple cubic | all (hkl) |
| BCC | $h + k + l = \text{even}$ |
| FCC | h, k, l all odd or all even |

Example: X-ray diffraction of Tungsten

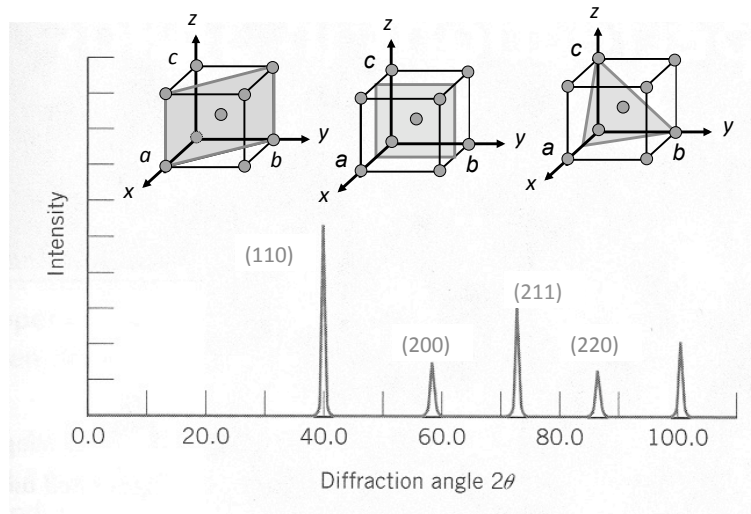
$\lambda = 0.1542\text{nm}$, BCC tungsten, $R=0.137\text{nm}$

Index each of the peaks



BCC: $h+k+l$ even, $a = 4R/\sqrt{3}$

Example: X-ray diffraction of Tungsten



BCC: $h+k+l$ even, $a = 4R/\sqrt{3}$