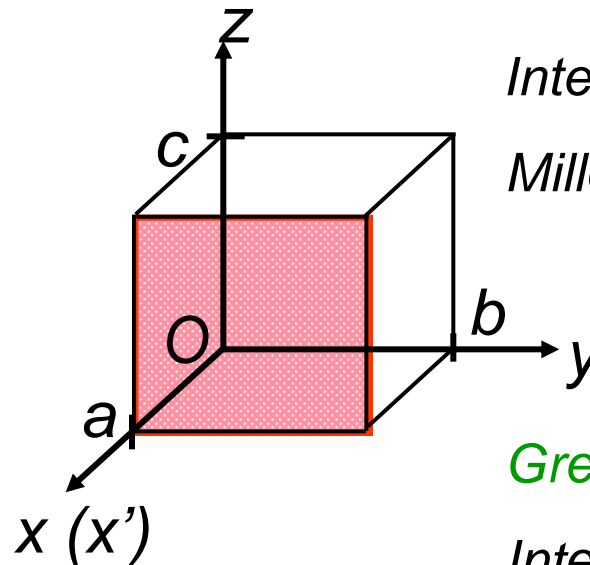
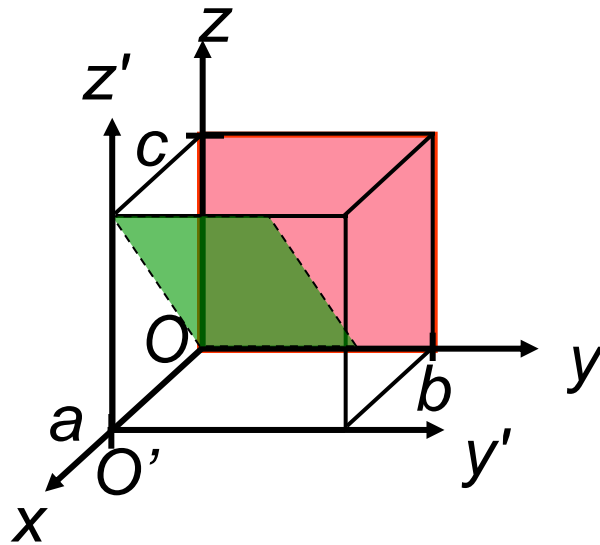


Chapter 3: The Structure of Crystalline Solids (3)

Additional Notes (1)

- For a crystal plane that passes through the origin, to determine the Miller Indices, a new origin or a parallel plane **that is equivalent** needs to be selected



Pink plane

Intercepts $1 \infty \infty$

Miller index (100)

Green plane

Intercepts $-1 \infty 1$

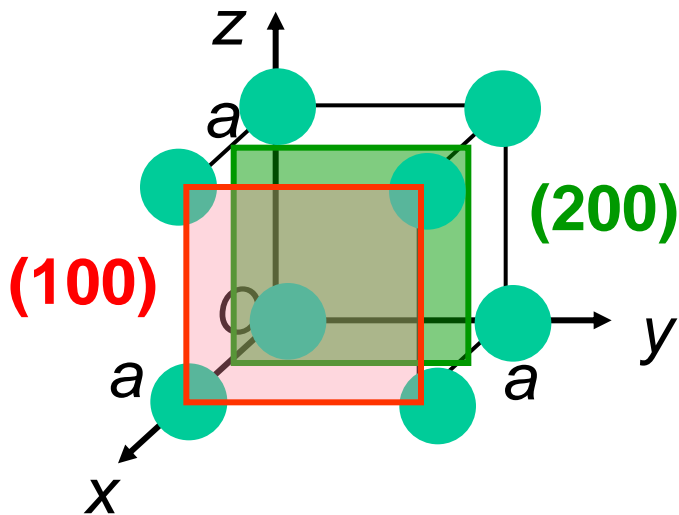
Miller index $(\bar{1}01)$



Chapter 3: The Structure of Crystalline Solids (3)

Additional Notes (2)

- Indices for planes with integer indices often **can NOT be reduced**. For example, for simple cubic lattice
 - (200) (green) plane does NOT pass through any atoms center
 - (100) plane passes through atoms centers
 - (200) and (100) planes, in this case, strictly speaking, are NOT geometrically equivalent



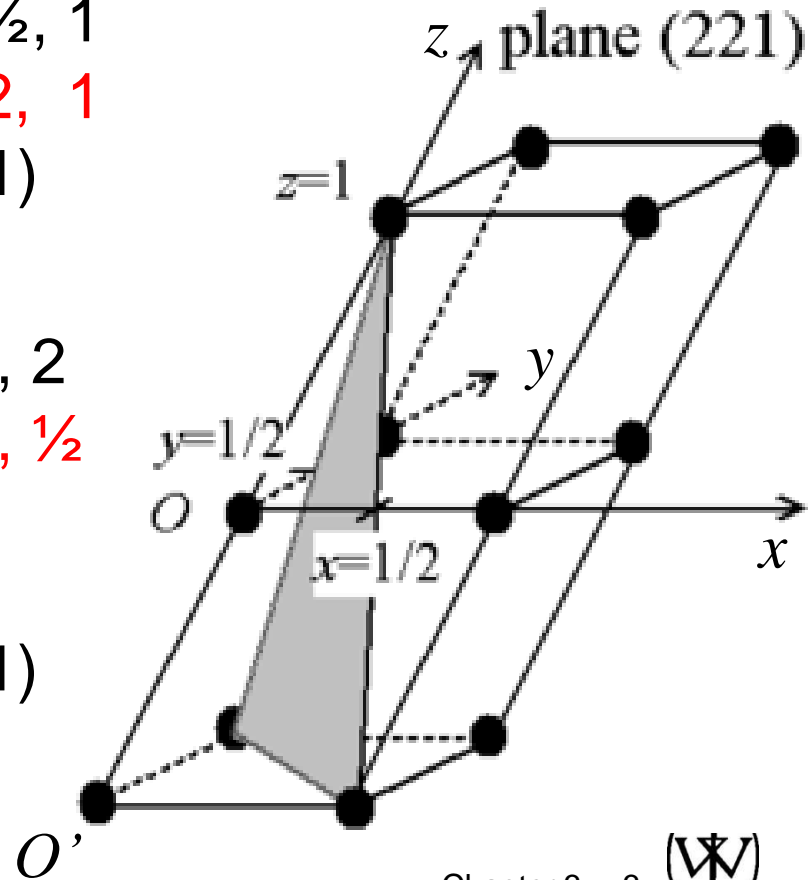
Chapter 3: The Structure of Crystalline Solids (3)

Additional Notes (3): after obtaining inverse for the intercepts for axes, **multiplication** by common integer **OK**

Example 1: shaded plane

- If choose origin at O,
Three intercepts will be $\frac{1}{2}, \frac{1}{2}, 1$
Corresponding reciprocals be $2, 2, 1$
Resulting Miller Indices will be (221)

- If choose origin at O',
Three intercepts will be $1, 1, 2$
Corresponding reciprocal be $1, 1, \frac{1}{2}$
Multiple by smallest common integer (i.e., 2) to remove fraction
Resulting Miller indices will be (221)



Chapter 3: The Structure of Crystalline Solids (3)

Additional Notes (3'): after obtaining inverse for intercepts for axes, **multiplication** by common integer OK

Example 2: shaded plane

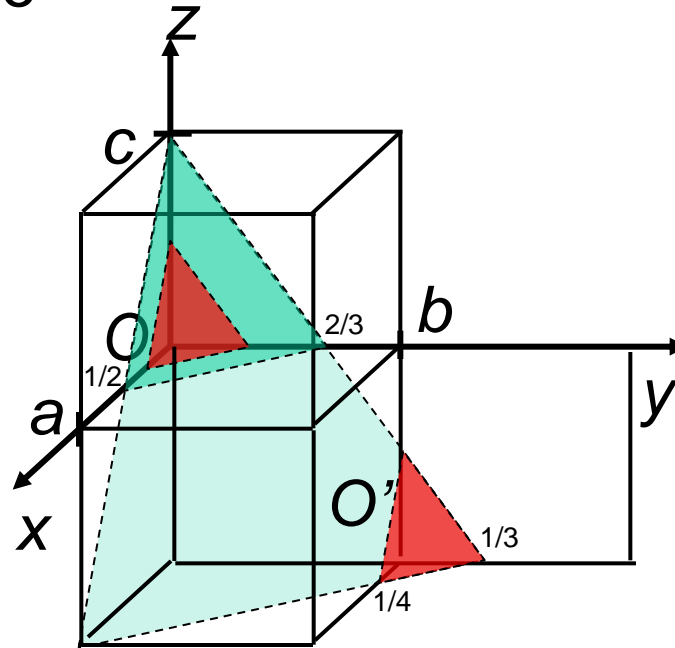
- If choose origin at O,
Three intercepts will be
Corresponding reciprocals be
Multiply by common integer (2 here) to remove fraction
Resulting Miller Indices will be (432)

$\frac{1}{2}, \frac{2}{3}, 1$
 $2, \frac{3}{2}, 1$

- Then, for the (432) plane
Three intercepts will be $\frac{1}{4}, \frac{1}{3}, \frac{1}{2}$
The plane appears to be “different”:

- it appears to be the red-shaded plane instead of original green-shaded plane?!

Extend that plane & the equivalency would appear!



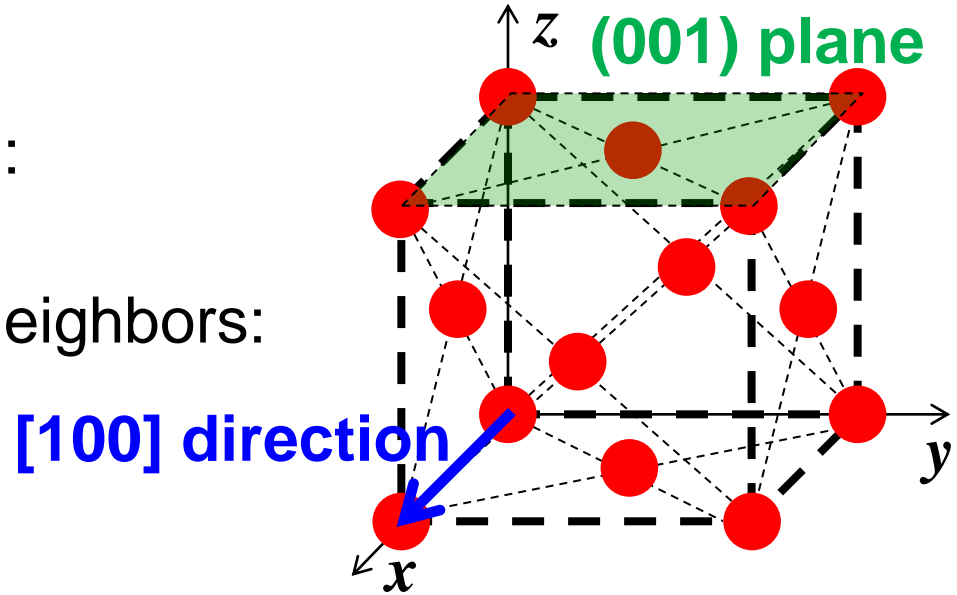
Class Exercise

- Draw face centered cubic (FCC) lattice structures and label the axis
- Give coordination number (CN) for atoms in the FCC structure
- Give the average number of atoms in a unit cell for FCC structure and explain why
- Given atoms radius of R for the FCC structure, do the followings:
 - Calculate distance between the centers of one atom to the center of its nearest neighbor
 - FCC cubic unit cell edge length
 - Label [100] direction and (001) plane
 - Calculate atomic packing factor for FCC
 - Calculated theoretical density if atomic mass is A and Avergado number is N_A



Class Exercise

- CN = 12
- Number of atoms in unit cell:
 $8 \times (1/8) + 6 \times (1/2) = 4$
- Distance between nearest neighbors:
 $2R$
- FCC unit cell edge length:
 $2\sqrt{2}R$



- Atomic packing factor

$$APF = \frac{4 \cdot \frac{4}{3} \pi R^3}{(2\sqrt{2}R)^3} = \frac{\pi}{3\sqrt{2}} \approx 0.74$$

- Theoretical density:

$$\rho_{theo} = \frac{4 \frac{A}{N_A}}{(2\sqrt{2}R)^3} = \frac{A}{4\sqrt{2}R^3 N_A}$$



Close Packed Direction & Close Packed Planes

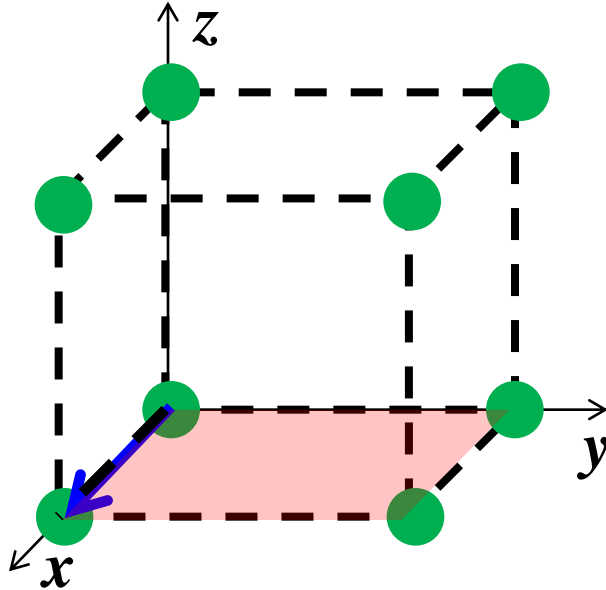
- For a crystal structure, there exist certain directions and planes in which atoms are packed at highest (linear or planar) density within that structure

	Close packed direction	Close packed plane
Simple cubic	$\langle 100 \rangle$	NO, but $\{100\}$ has highest planar density
BCC	$\langle 111 \rangle$	NO, but $\{110\}$ has highest planar density
FCC	$\langle 110 \rangle$	$\{111\}$



Close Packed Direction & Planes of Highest Planar Density in Cubic Crystals

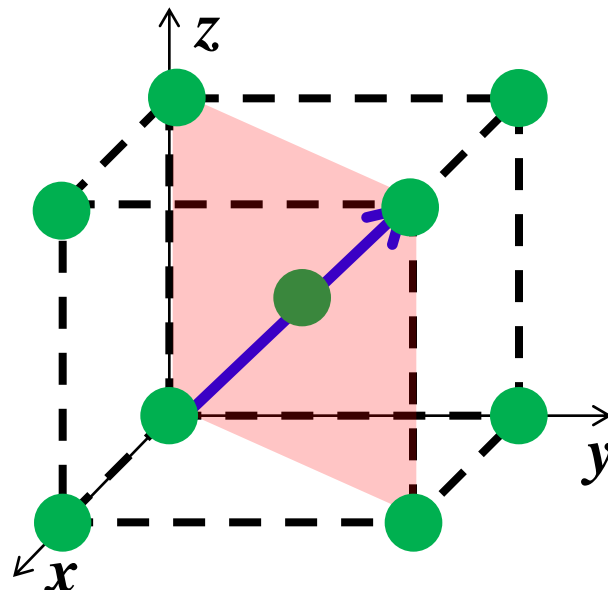
Simple Cubic



$\langle 100 \rangle$

$\{100\}$

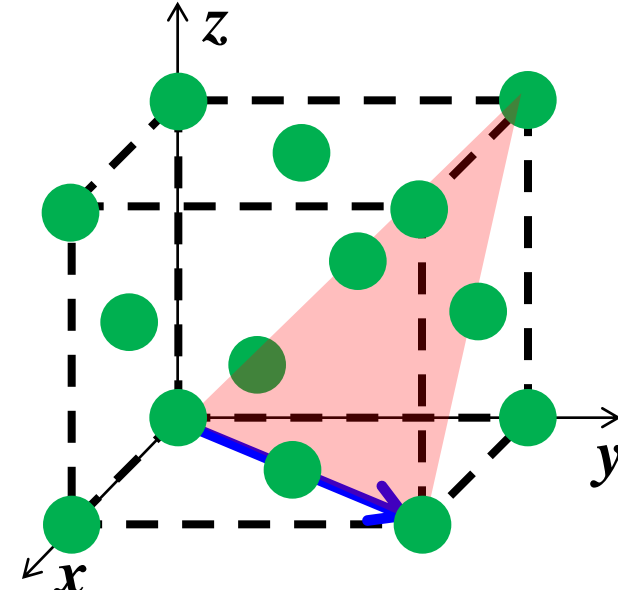
BCC



$\langle 111 \rangle$

$\{110\}$

FCC



$\langle 110 \rangle$

$\{111\}$

Close Packed Direction

Plane with Highest Planar Density

Also close packing plane



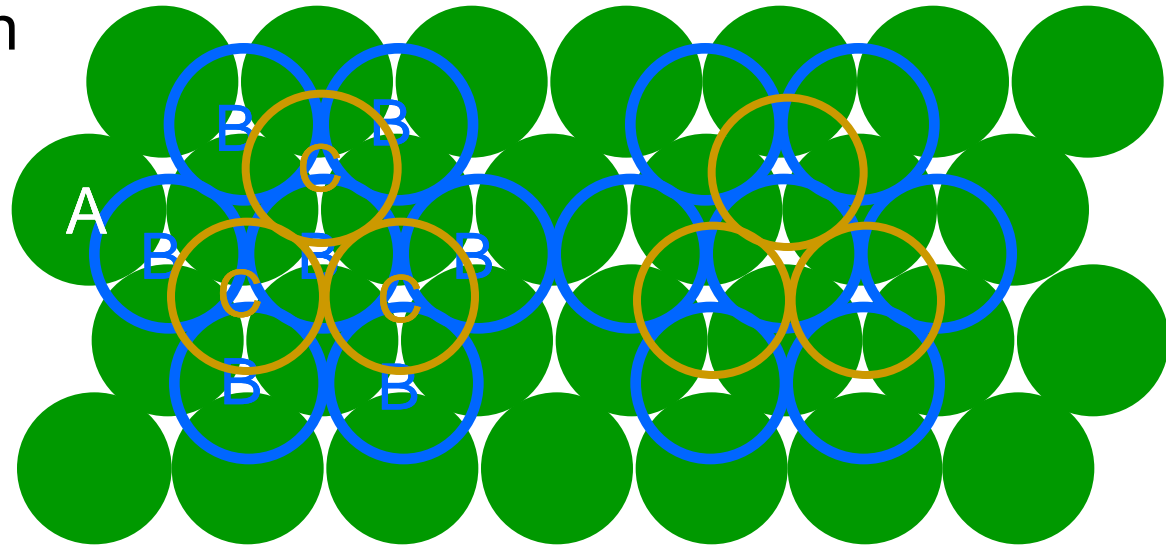
Close Packing in FCC Crystal

- ABCABC... Stacking Sequence
- 2D Projection

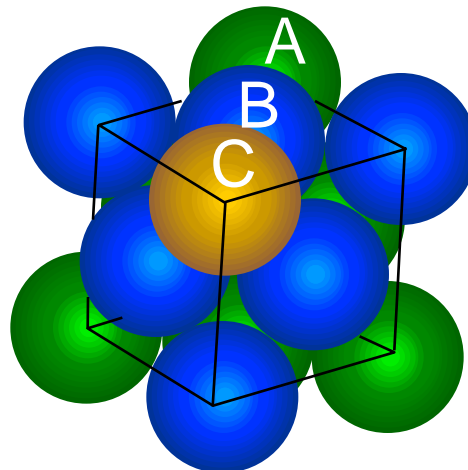
A sites

B sites

C sites

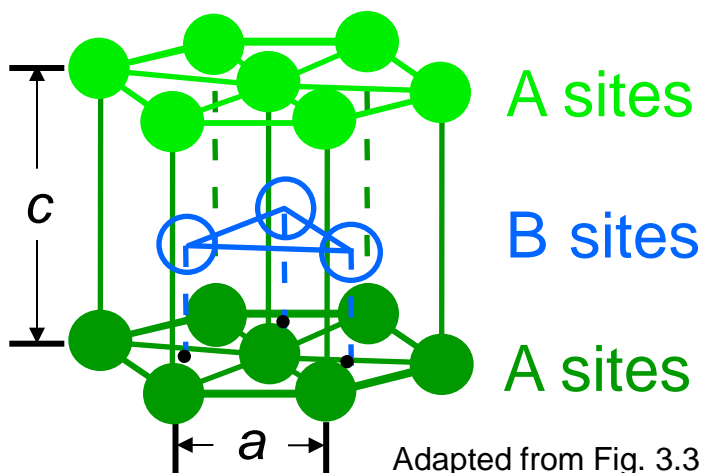


- FCC Unit Cell



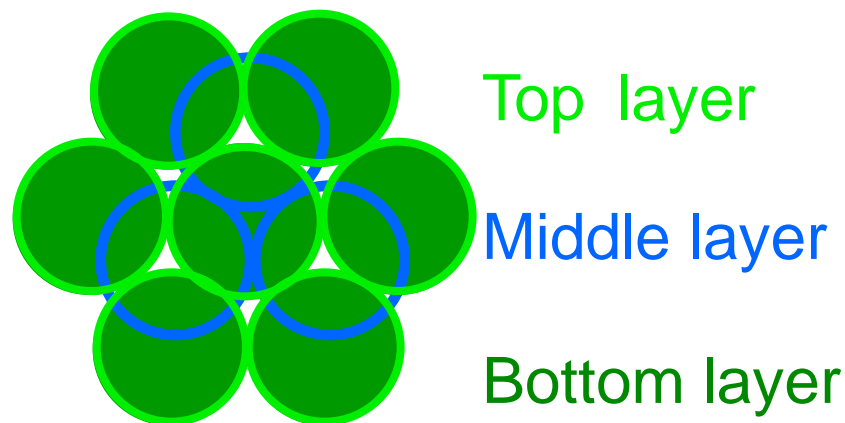
Hexagonal Close-Packed (HCP) Structure

- ABAB... Stacking Sequence
- 3D Projection



Adapted from Fig. 3.3(a),
Callister & Rethwisch 8e.

- 2D Projection



- CN = 12
- APF = 0.74
- $c/a = 1.633$

6 atoms/unit cell

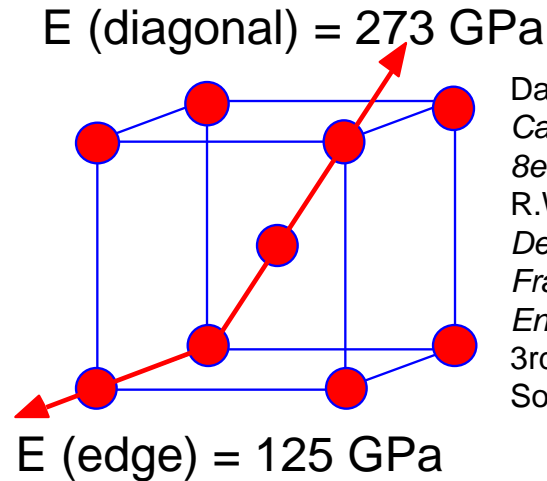
ex: Cd, Mg, Ti, Zn



Anisotropy in Crystals

- Single Crystals

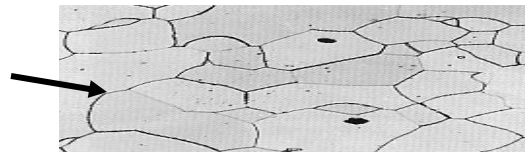
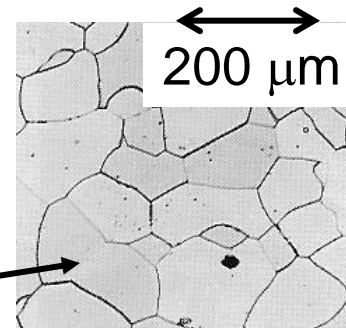
- Properties vary with direction: **anisotropic**.
- Example: the modulus of elasticity (E) in BCC iron:



Data from Table 3.3, *Callister & Rethwisch 8e*. (Source of data is R.W. Hertzberg, *Deformation and Fracture Mechanics of Engineering Materials*, 3rd ed., John Wiley and Sons, 1989.)

- Polycrystals

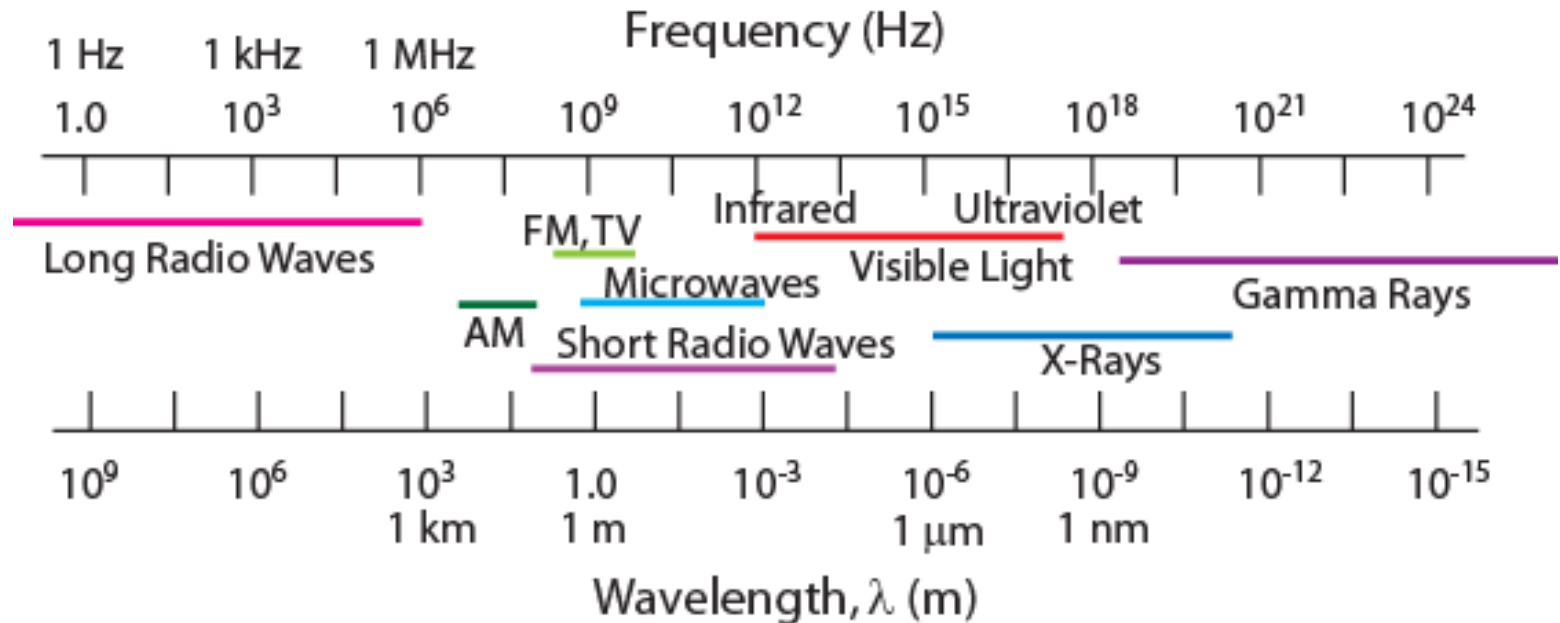
- Properties may/may not vary with direction.
- If grains are randomly oriented: **isotropic**.
($E_{\text{poly iron}} = 210 \text{ GPa}$)
- If grains are elongated along certain directions (**textured**), then anisotropic.



Adapted from Fig. 4.14(b), *Callister & Rethwisch 8e*. (Fig. 4.14(b) is courtesy of L.C. Smith and C. Brady, the National Bureau of Standards, Washington, DC [now the National Institute of Standards and Technology, Gaithersburg, MD].)

Crystal Structure Determination via X-Ray Diffraction

Electromagnetic Spectrum

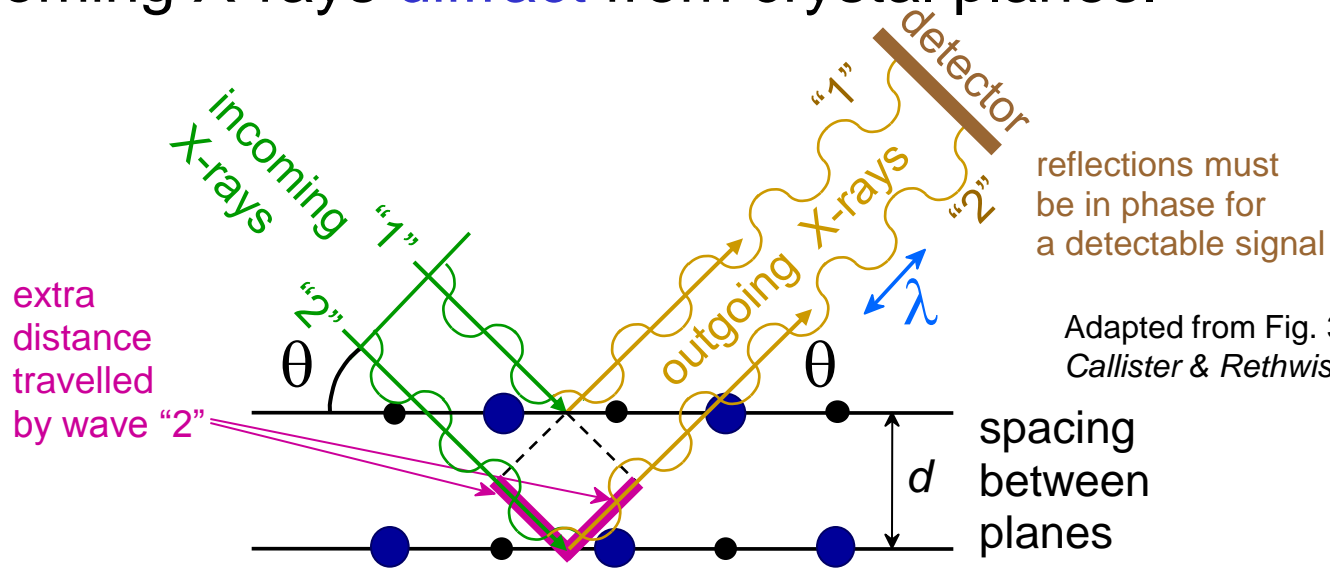


- Diffraction gratings must have spacings comparable to the wavelength of diffracted radiation.
- Can't resolve spacings $< \sim \lambda$
- Spacing is the distance between parallel planes of atoms.



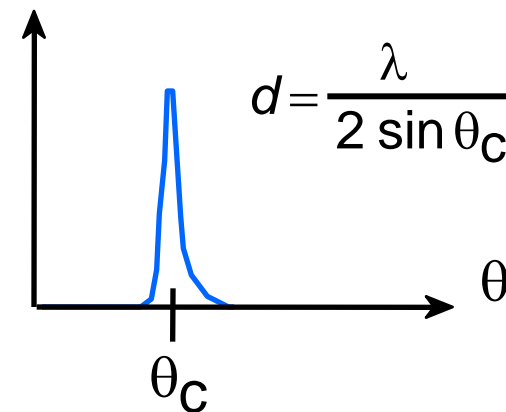
X-Rays Diffraction to Determine Crystal Structure

- Incoming X-rays diffract from crystal planes.

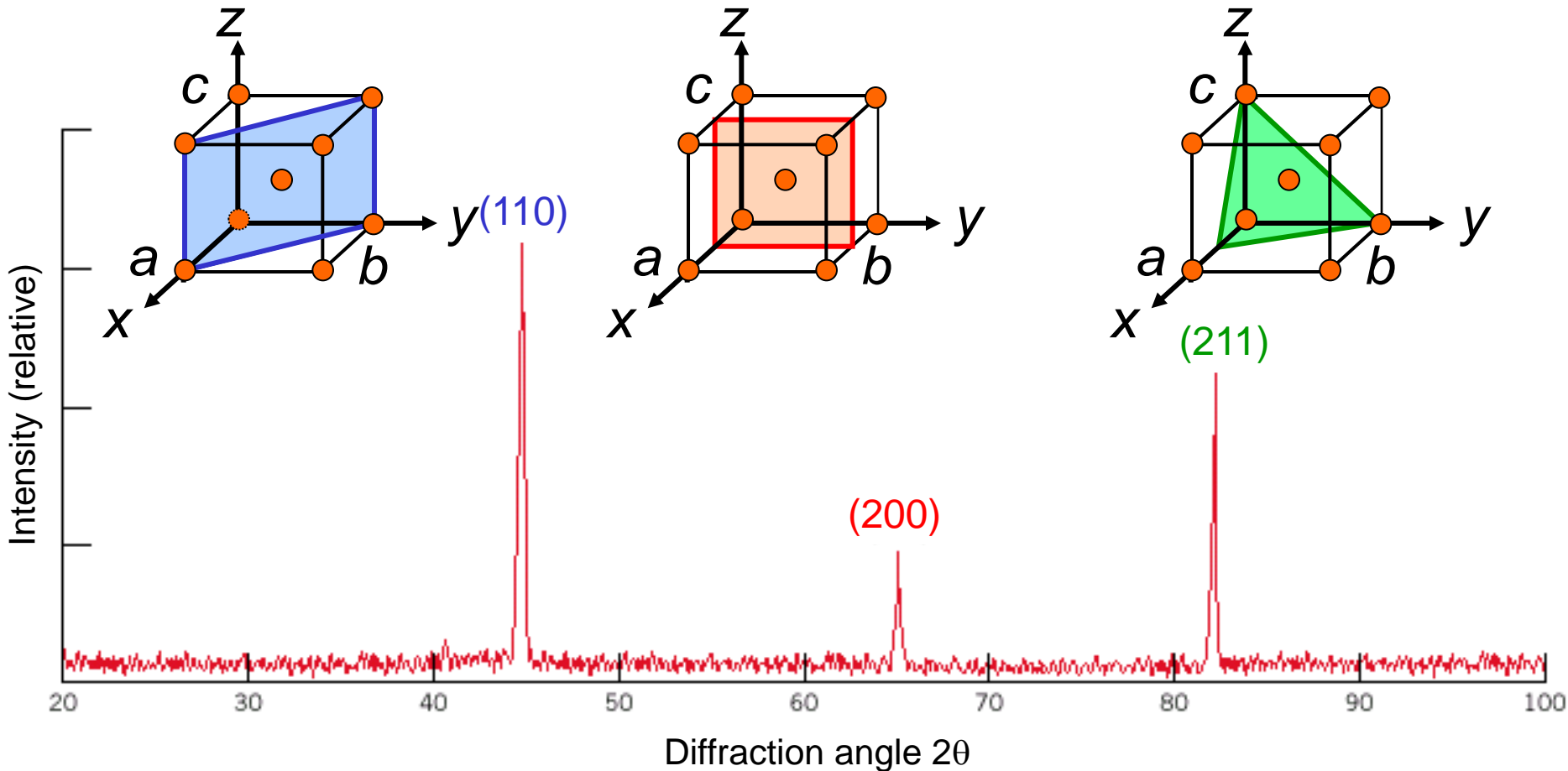


- Measurement of critical angle, θ_c , allows computation of planar spacing, d .
- Appearance of peaks allow structure determination

X-ray intensity (from detector)



Example of X-Ray Diffraction Pattern



Diffraction pattern for polycrystalline α -iron (BCC)

Adapted from Fig. 3.22, *Callister 8e*.

SUMMARY

- Crystalline vs. amorphous materials
- Single crystal vs. polycrystalline materials
- Crystal structure – atoms periodic arrangement in crystals
- Lattice, unit cell, coordination number
- Crystal systems
- Basic unit cell structure for cubic crystal systems: simple cubic, face-centered cubic, body-centered cubic
- Point coordinates, directions, and planes in crystals and their indices
- Application problems: theoretical density, atomic packing factor, linear density, and planar density
- Structure determination by X-ray diffraction



Homework Chapter 3

- **Read chapter 3 (omit the sections on Hexagonal crystals) and give a statement firming you finish the reading**
- Calister 8ed, 3.8; 3.23; 3.31; 3.41; one additional problem (see the end)

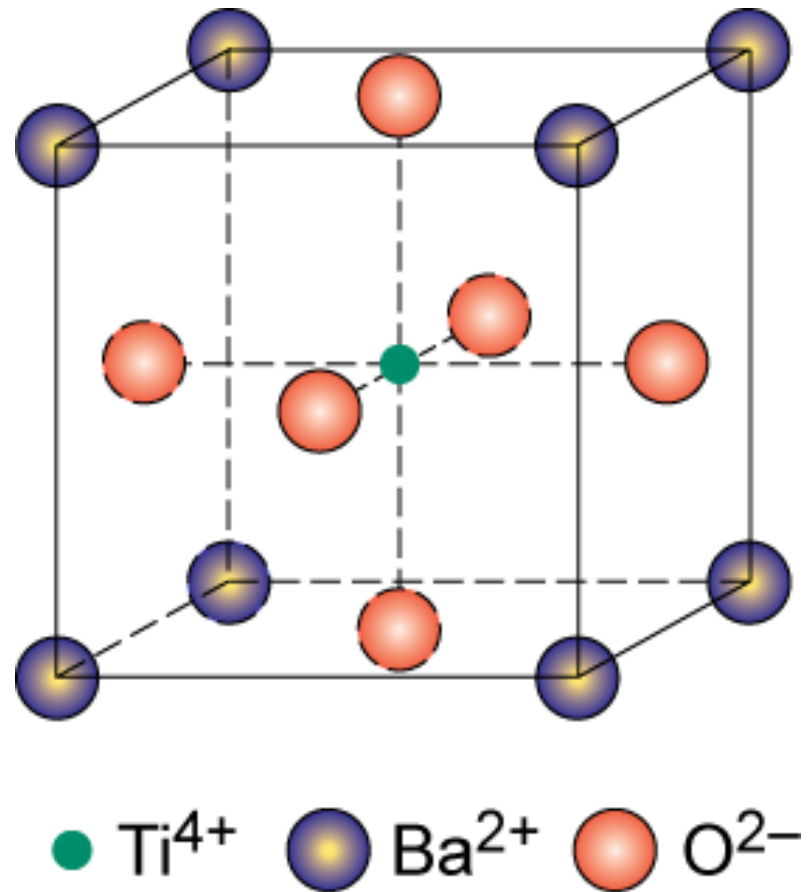


- Calister 8ed, 3.8

Calculate the radius of an iridium atom, given that Ir has an FCC crystal structure, a density of 22.4 g/cm³, and an atomic weight of 192.2 g/mol.



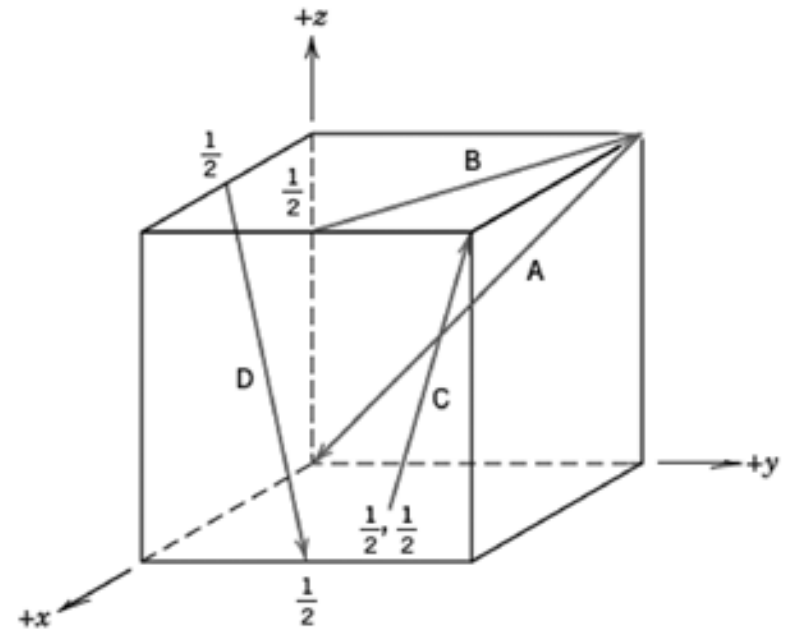
- Calister 8ed, 3.23
List the point coordinates of the titanium, barium, and oxygen ions for a unit cell of the BaTiO_3 perovskite crystal structure (Figure 12.6).



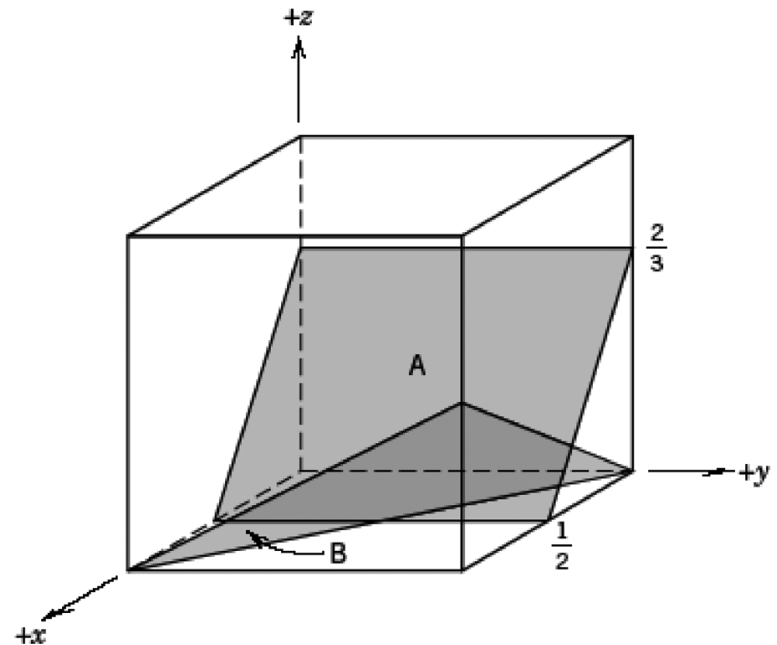
Adapted from Fig. 12.6,
Callister & Rethwisch 8e.



- Calister 8ed, 3.31
Determine the indices for the directions shown in the following cubic unit cell:



- Calister 8ed, 3.41
Determine the Miller indices for the planes shown in the following unit cell



Additional Homework

- Draw body centered cubic (BCC) lattice structures and label the axis
- Give coordination number (CN) for atoms in the BCC structure
- Give the average number of atoms in a unit cell for BCC structure and explain why
- Given atoms radius of R for the BCC structure, do the followings:
 - Calculate distance between the centers of one atom to the center of its nearest neighbor
 - BCC cubic unit cell edge length
 - Label [100] direction and (001) plane
 - Calculate atomic packing factor for BCC
 - Calculated theoretical density if atomic mass is A and Avergado number is N_A

