CRYSTAL STRUCTURES OF SOLIDS

A PART OF

B.Sc. Physics (Hons.) Old syllabus: Paper-IX

B.Sc. Physics (Hons.) Semester: V (CBCS); Course: CC-XII

DR. SHYAMSUNDAR GHOSH

Assistant Professor,

Department of Physics,

Bejoy Narayan Mahavidyalaya,

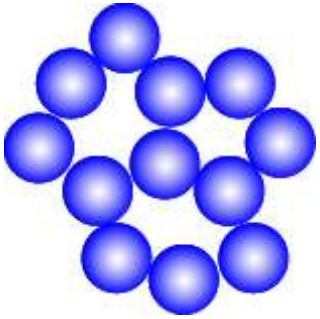
Hooghly-712147

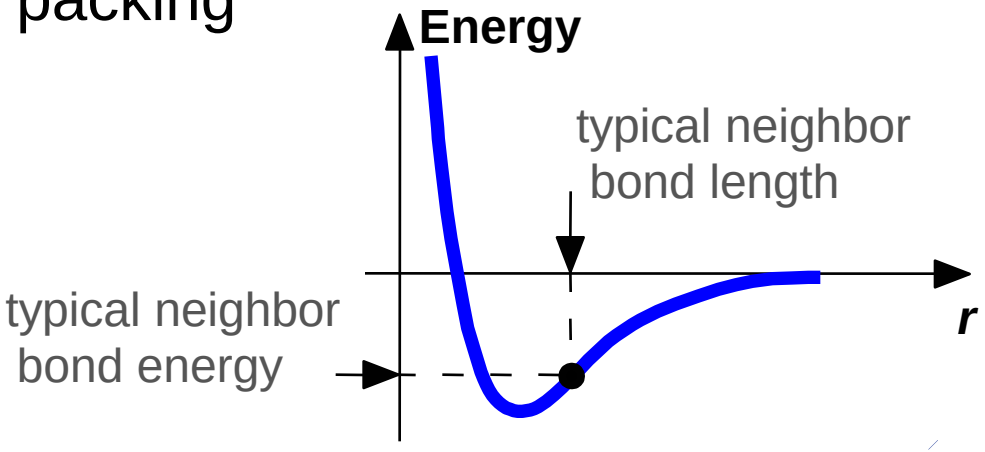
Question…..?

- When all the metals are known to be crystalline and have metallic bonding then why different metals exhibit different properties (e.g. Density, strength, etc.)……..?
- Many questions about metal can be answered by knowing their **Crystal STRUCTURE** (the arrangement of the atoms within the metals).

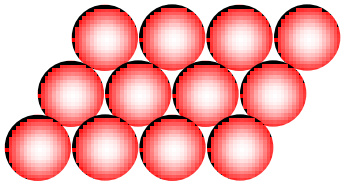
Energy and Packing

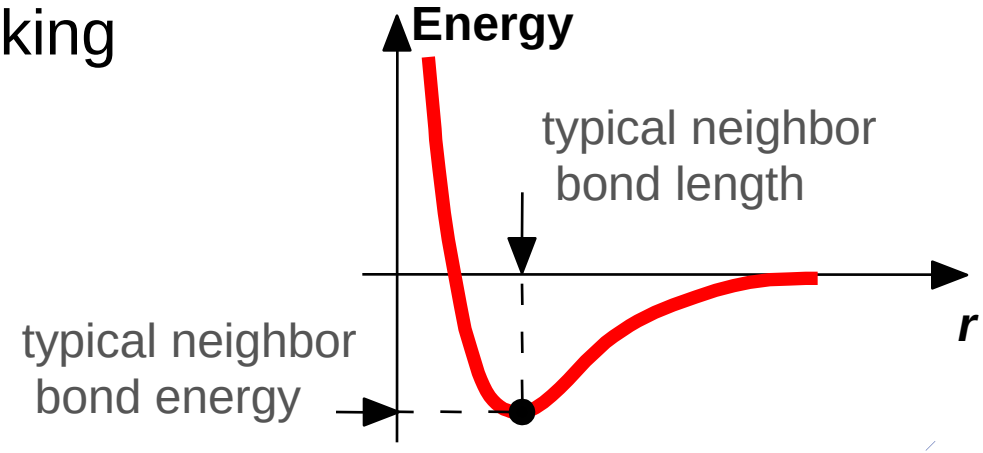
- Non dense, random packing





- Dense, ordered packing



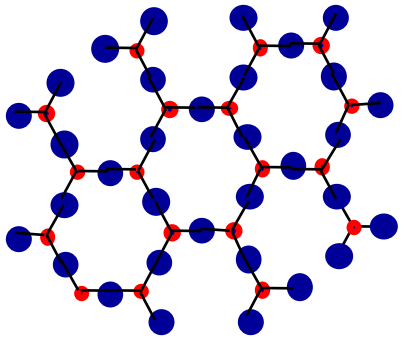


Dense, ordered packed structures tend to have lower energies.

Materials and Packing

Crystalline materials...

- atoms pack in periodic, 3D arrays
- typical of: -metals
  -many ceramics
  -some polymers



crystalline SiO_2

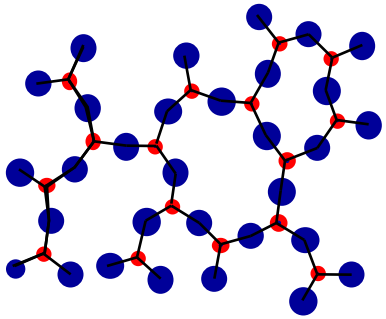
Adapted from Fig. 3.40(a), *Callister & Rethwisch 3e.*

• **Si** ● **Oxygen**

Noncrystalline materials...

- atoms have no periodic packing
- occurs for: -complex structures
  -rapid cooling

"Amorphous" = Noncrystalline



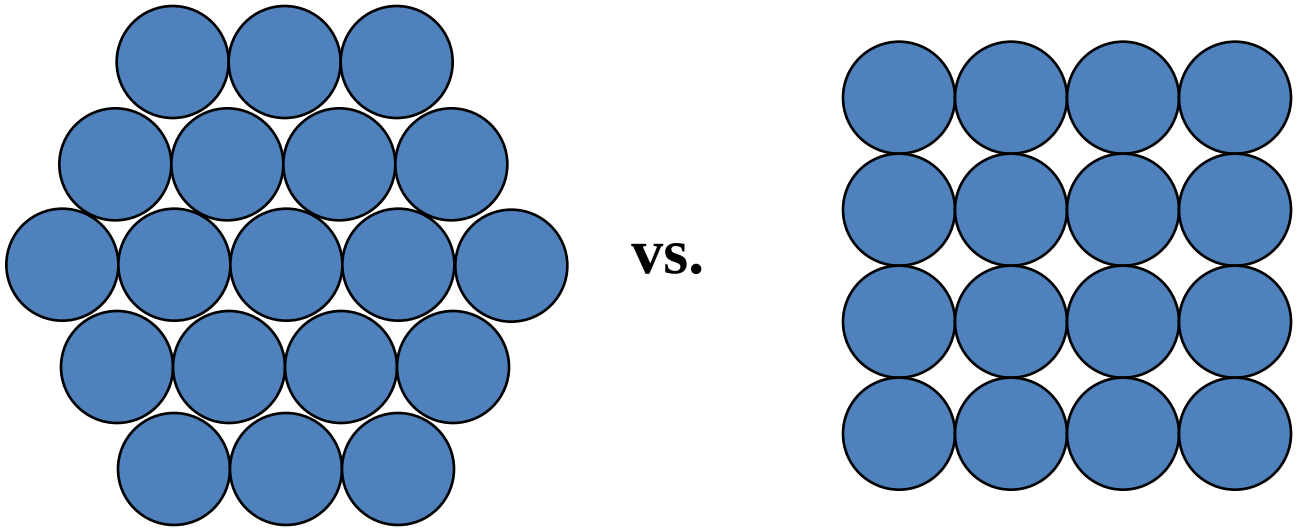
noncrystalline SiO_2

Adapted from Fig. 3.40(b), *Callister & Rethwisch 3e.*

Metallic Crystal Structures

- How can we stack metal atoms to minimize empty space?

2 - Dimensions



Now stack these 2-D layers to make 3-D structures

Metallic Crystal Structures

- Tend to be densely packed.
- Reasons for dense packing:
  - Typically, only one element is present, so all atomic radii are the same.
  - Metallic bonding is not directional.
  - Nearest neighbor distances tend to be small in order to lower bond energy.
  - Electron cloud shields cores from each other
- Have the simplest crystal structures.

SOME DEFINITIONS …

- Lattice: 3D array of regularly spaced points
- Crystalline material: atoms situated in a repeating 3D periodic array over large atomic distances
- Amorphous material: material with no such order
- Hard sphere representation: atoms denoted by hard, touching spheres
- Reduced sphere representation
- Unit cell: basic building block unit (such as a flooring tile) that repeats in space to create the crystal structure

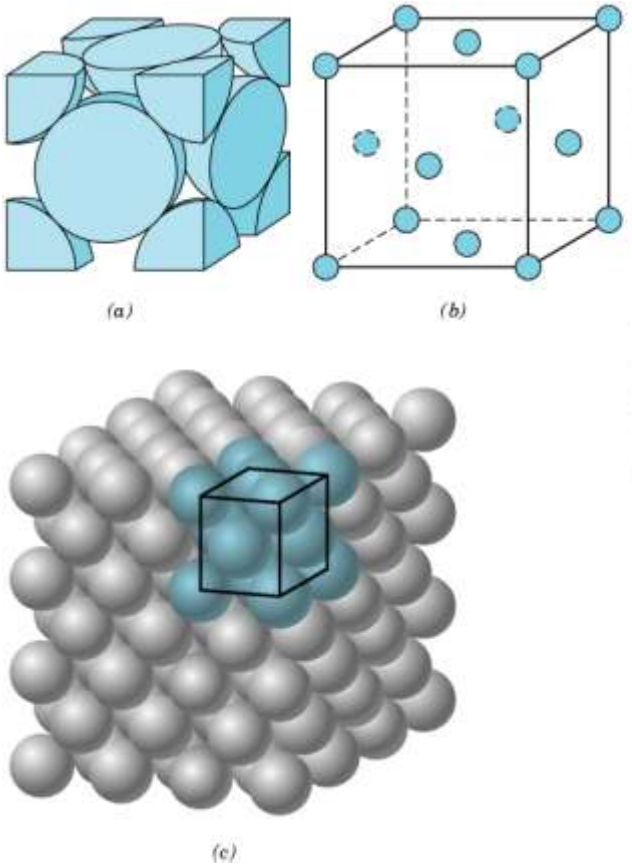


FIGURE 3.1 For the face-centered cubic crystal structure: (*a*) a hard sphere unit cell representation, (*b*) a reduced-sphere unit cell, and (*c*) an aggregate of many atoms. (Figure *c* adapted from W. G. Moffatt, G. W. Pearsall, and J. Wulff, *The Structure and Properties of Materials*, Vol. I, *Structure*, p. 51. Copyright © 1964 by John Wiley & Sons, New York. Reprinted by permission of John Wiley & Sons, Inc.)

CRYSTAL SYSTEMS

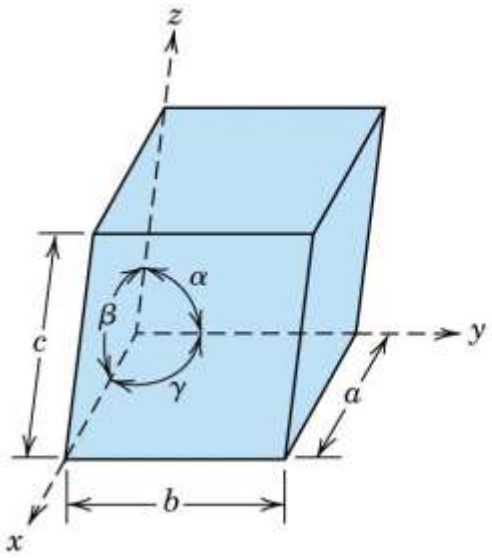
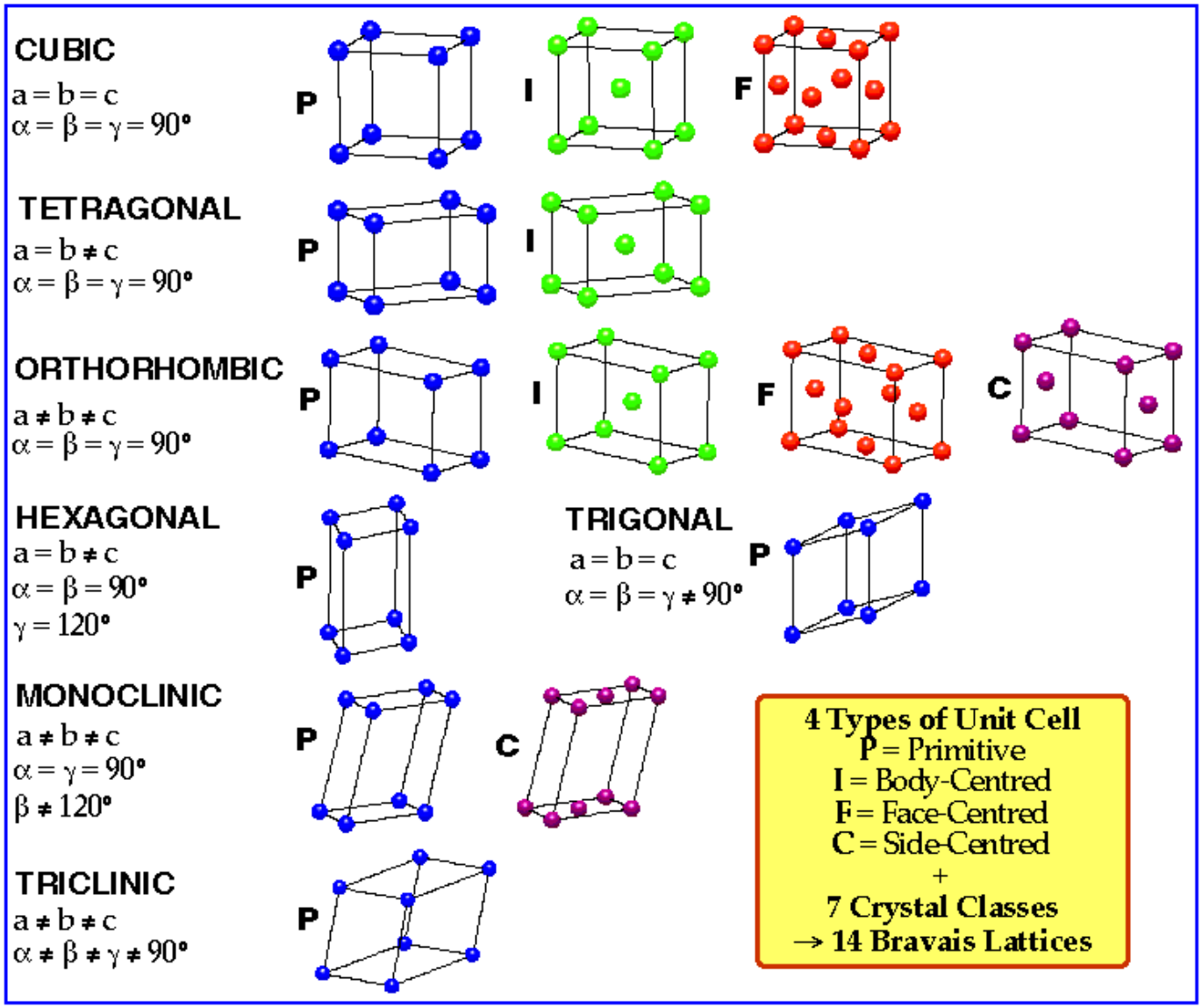


FIGURE 3.4 A unit cell with x, y, and z coordinate axes, showing axial lengths (a, b, and c) and interaxial angles (α, β, and γ).

- Based on shape of unit cell ignoring actual atomic locations
- Unit cell = 3-dimensional unit that repeats in space
- Unit cell geometry completely specified by *a, b, c* & α, β, γ ***(lattice parameters*** *or* ***lattice constants)***
- Seven possible combinations of *a, b, c* & α, β, γ, resulting in seven crystal systems

CRYSTAL SYSTEMS

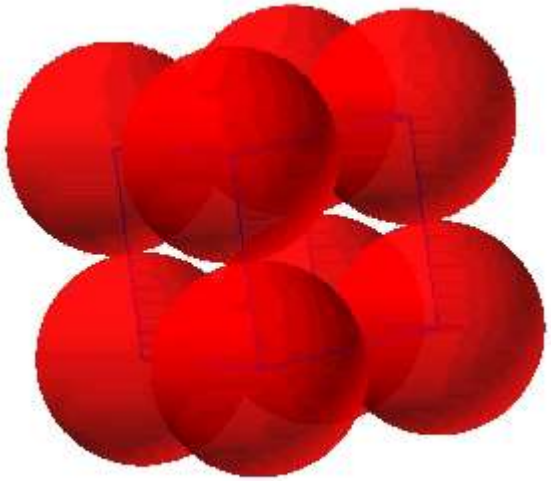


The Crystal Structure of Metals

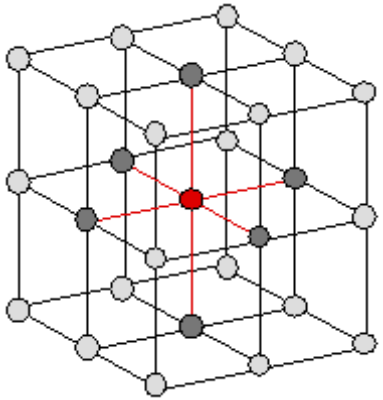
- Metals and Crystals
  - What determines the strength of a specific metal.
- Four basic atomic arrangements

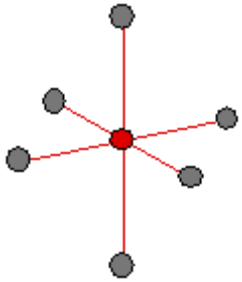
Simple Cubic Structure (SC)

- Rare due to low packing density (only Po has this structure)
- Close-packed directions are cube edges.



- Coordination # = 6
  (# nearest neighbors)



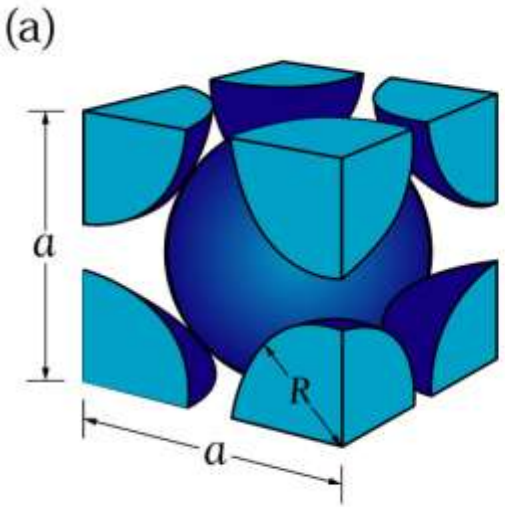


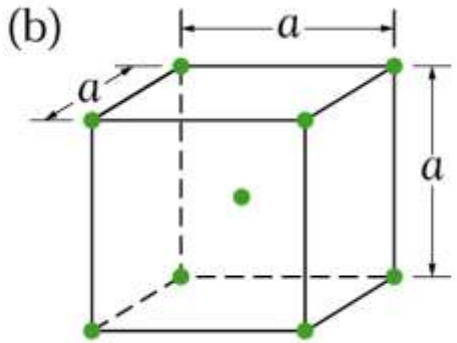
No. of atoms/unit cell : 8 corners x 1/8 = 1

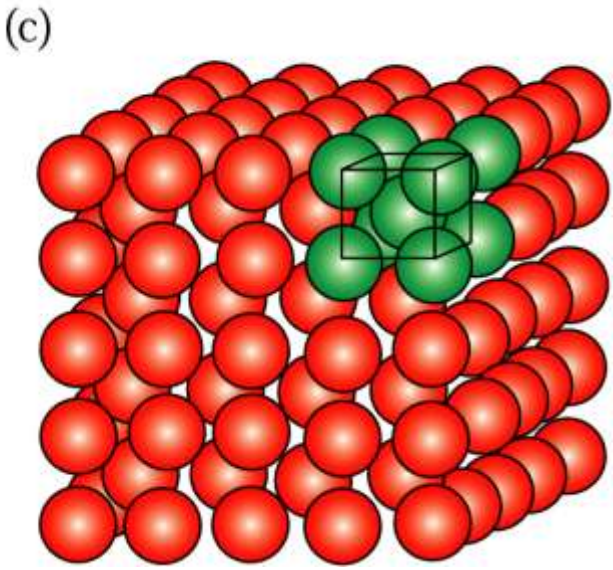
(Courtesy P.M. Anderson)

2of 4 basic atomic arrangements

2. Body-centered cubic (bcc)





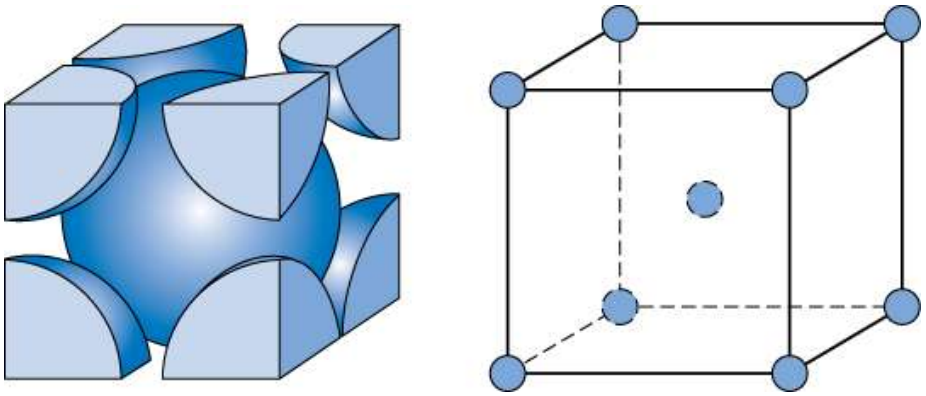


Body Centered Cubic Structure (BCC)

- Atoms touch each other along cube diagonals.
  --Note: All atoms are identical; the center atom is shaded differently only for ease of viewing.

ex: Cr, W, Fe (α), Tantalum, Molybdenum

- Coordination # = 8



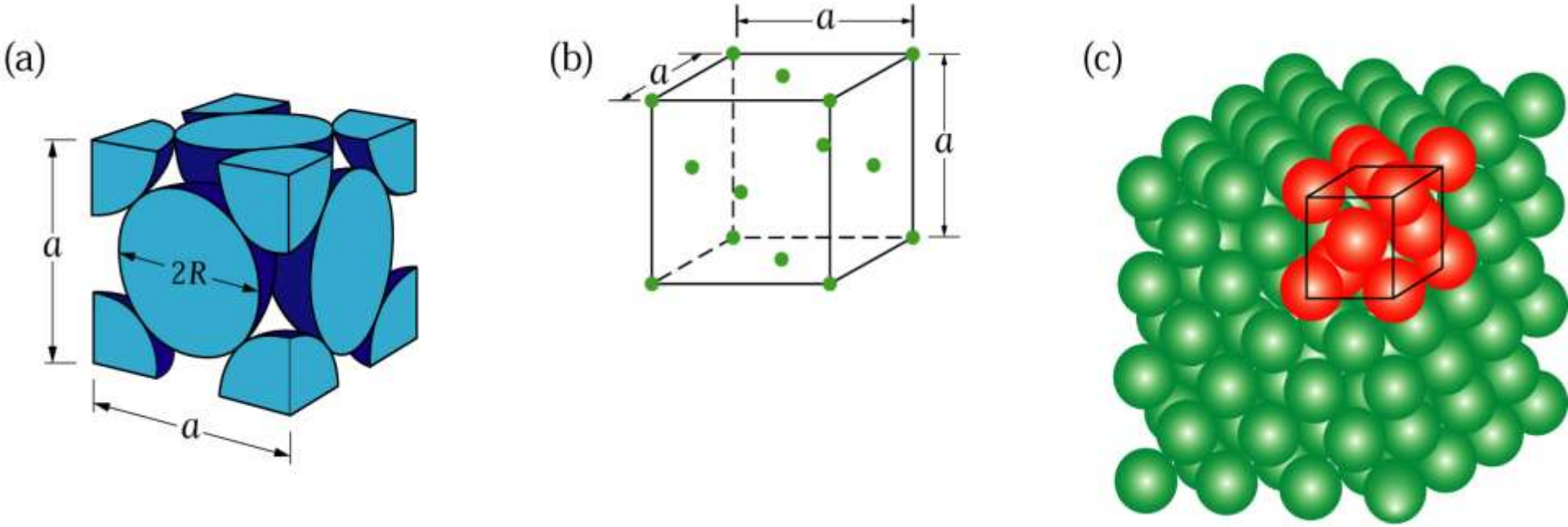
Adapted from Fig. 3.2,
Callister & Rethwisch 3e.

2 atoms/unit cell: 1 center + 8 corners x 1/8

(Courtesy P.M. Anderson)

3 of 4 basic atomic arrangements

3. Face-centered cubic (fcc) also known as Cubic close packing

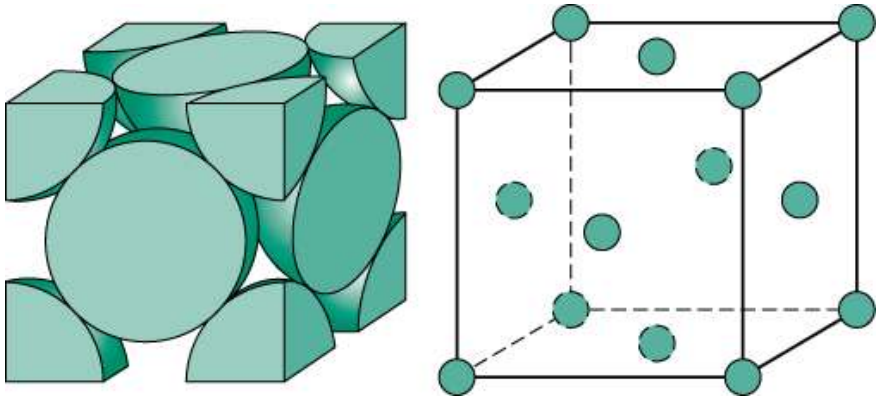


Face Centered Cubic Structure (FCC)

- Atoms touch each other along face diagonals.
  --Note: All atoms are identical; the face-centered atoms are shaded differently only for ease of viewing.

ex: Al, Cu, Au, Pb, Ni, Pt, Ag

- Coordination # = 12



Adapted from Fig. 3.1, *Callister & Rethwisch 3e.*

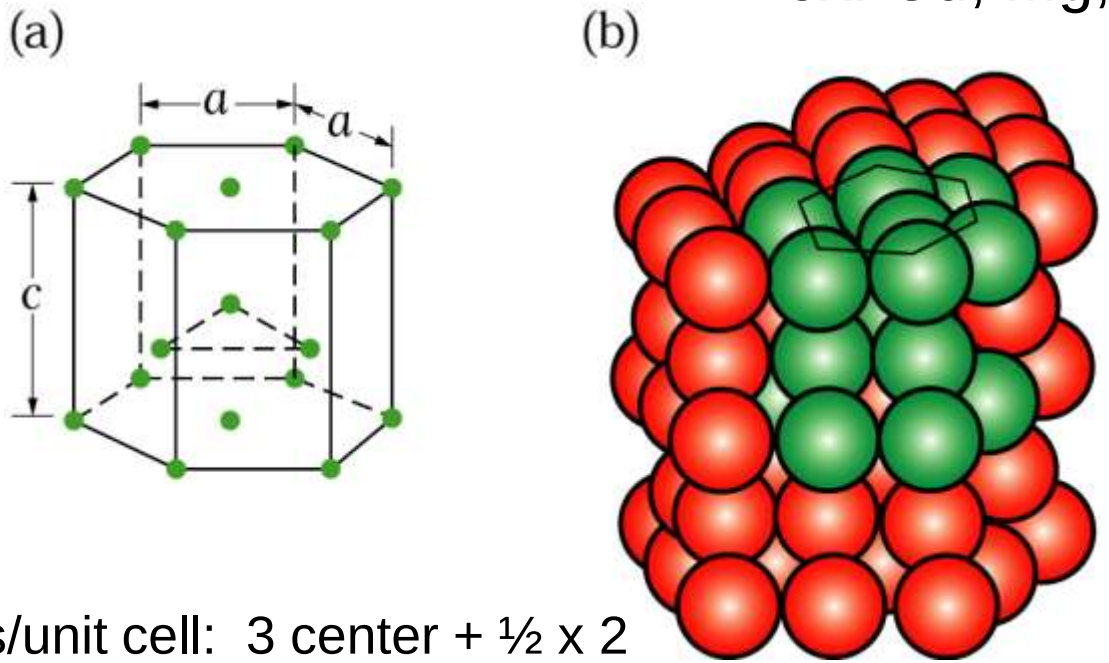
4 atoms/unit cell: 6 face x 1/2 + 8 corners x 1/8

(Courtesy P.M. Anderson)

4 of 4 basic atomic arrangements

4. Hexagonal close-packed (hcp)

ex: Cd, Mg, Ti, Zn

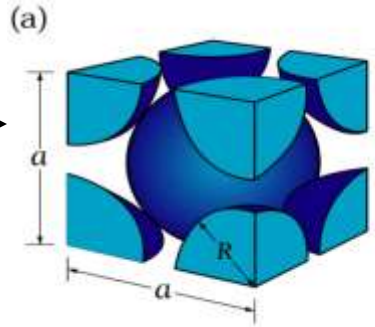


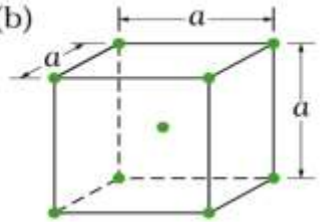
6 atoms/unit cell: 3 center + ½ x 2 top and bottom + 1/6 x 12 corners

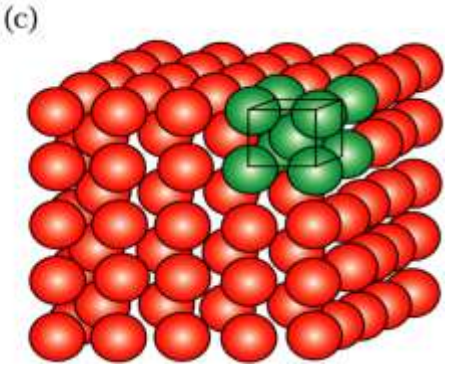
Coordination # = 12

Review of the three basic Atomic Structures

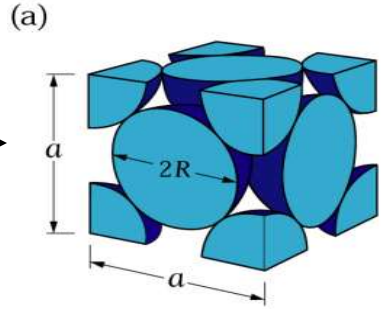
B.C.C.

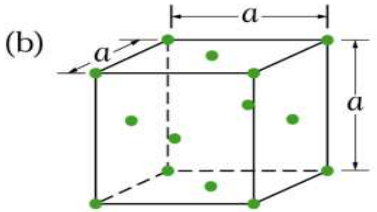


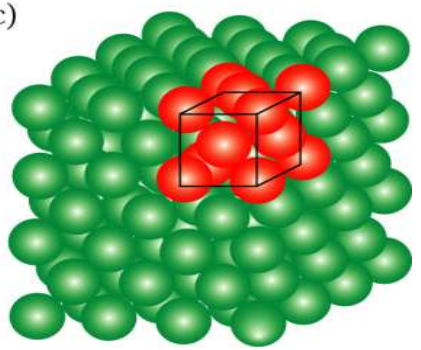




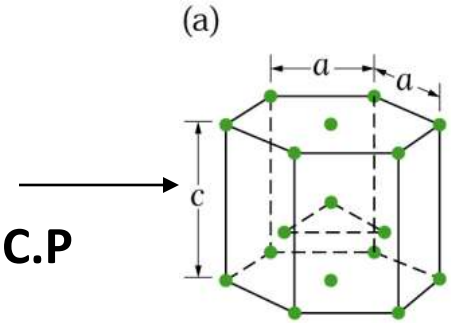
F.C.C

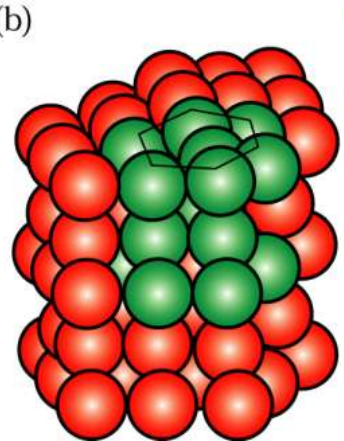






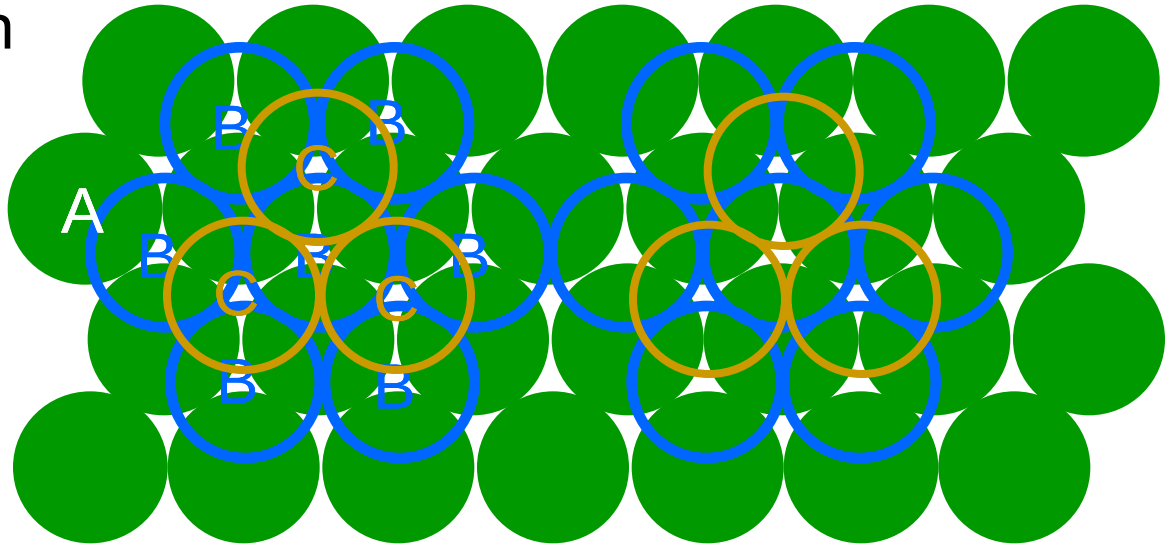
H.C.P



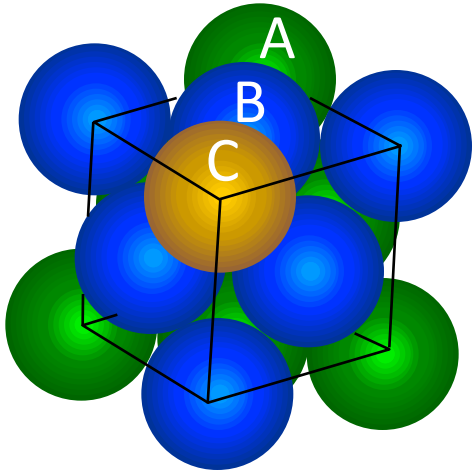


FCC Stacking Sequence

- ABCABC... Stacking Sequence
- 2D Projection

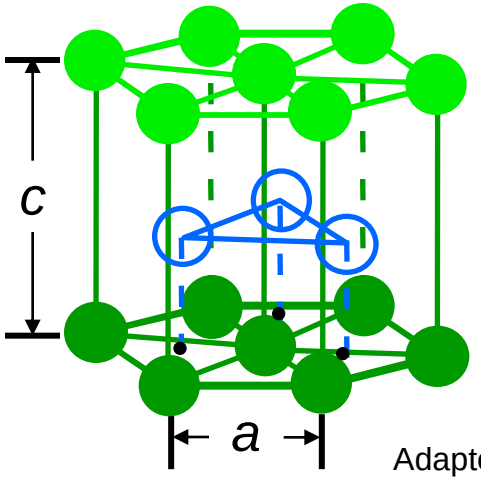


- FCC Unit Cell



Hexagonal Close-Packed Structure (HCP)

- ABAB... Stacking Sequence
- 3D Projection
- 2D Projection

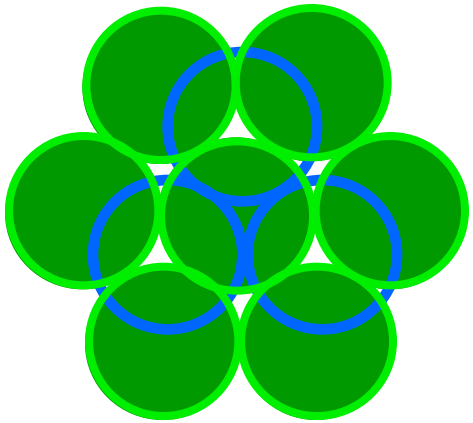


A sites

B sites

A sites

Adapted from Fig. 3.3(a), *Callister & Rethwisch 3e.*



Top layer

Middle layer

Bottom layer

ATOMIC PACKING FACTOR

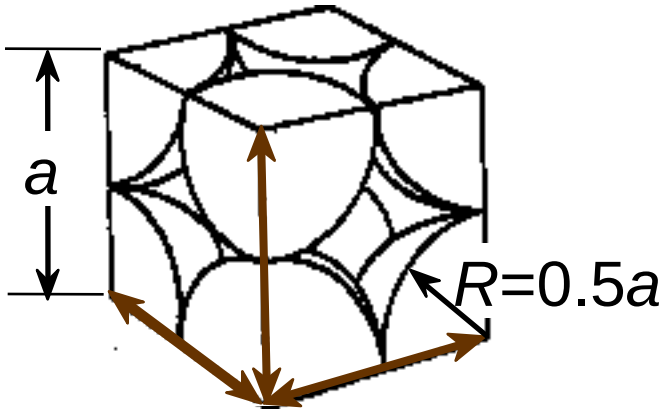
- Fill a box with hard spheres
  - Packing factor = total volume of spheres in box / volume of box
  - Question: what is the maximum packing factor you can expect?
- In crystalline materials:
  - Atomic packing factor = total volume of atoms in unit cell / volume of unit cell
  - (as unit cell repeats in space)

Atomic Packing Factor (APF)

$$APF = \frac{\text{Volume of atoms in unit cell*}}{\text{Volume of unit cell}}$$

*assume hard spheres

- APF for a simple cubic structure = 0.52



close-packed directions

contains 8 x 1/8 =

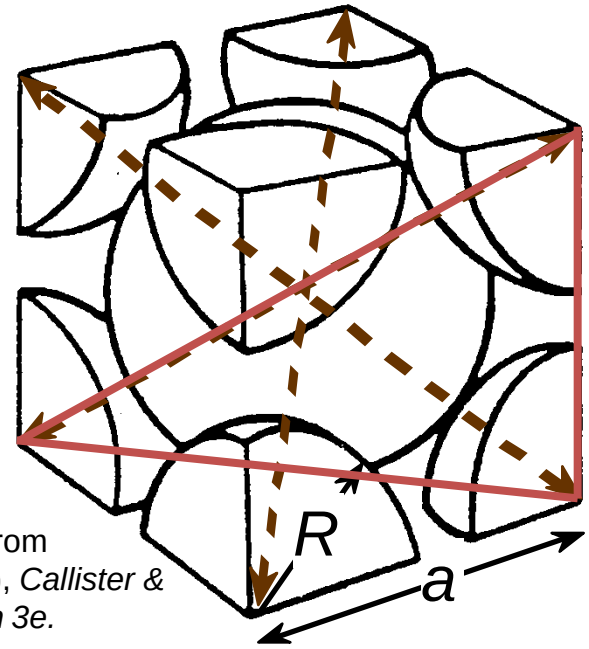
1 atom/unit cell

Adapted from Fig. 3.42, *Callister & Rethwisch 3e.*

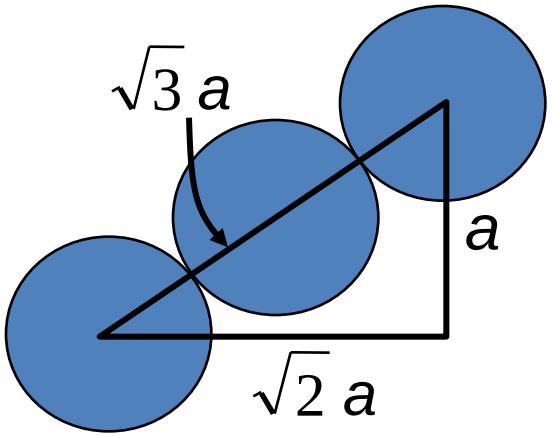
$$APF = \frac{\text{atoms}}{\text{unit cell}} \cdot \frac{\text{volume}}{\text{atom}} \Big/ \frac{\text{volume}}{\text{unit cell}} = \frac{1 \cdot \frac{4}{3}\pi (0.5a)^3}{a^3}$$

Atomic Packing Factor: BCC

- APF for a body-centered cubic structure = 0.68



Adapted from Fig. 3.2(a), *Callister & Rethwisch 3e.*

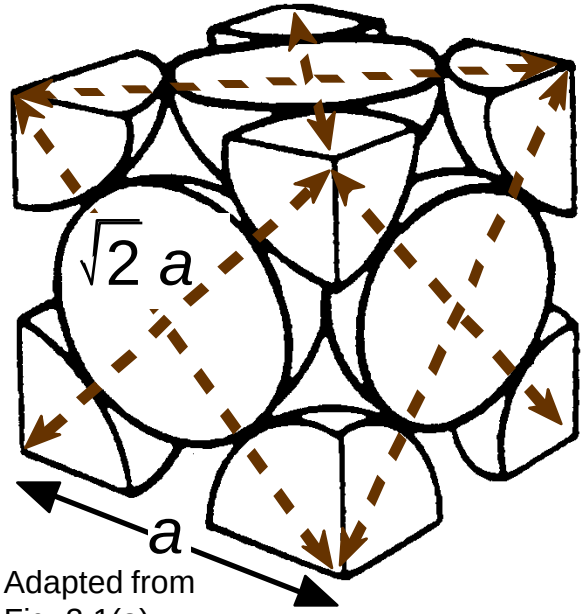


Close-packed directions:
length = $4R = \sqrt{3}\,a$

$$APF = \frac{\text{atoms}}{\text{unit cell}} \cdot \frac{\text{volume}}{\text{atom}} \Big/ \frac{\text{volume}}{\text{unit cell}} = \frac{2\left(\frac{4}{3}\pi\left(\frac{\sqrt{3}a}{4}\right)^3\right)}{a^3}$$

Atomic Packing Factor: FCC

- APF for a face-centered cubic structure = 0.74
  maximum achievable APF



Adapted from Fig. 3.1(a), *Callister & Rethwisch 3e.*

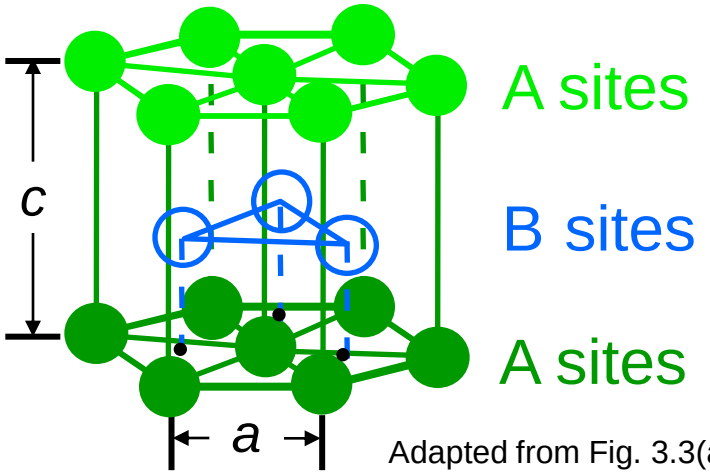
Close-packed directions:
length = $4R = \sqrt{2}\,a$

Unit cell contains:
6 x 1/2 + 8 x 1/8
= 4 atoms/unit cell

$$\text{APF} = \frac{\dfrac{\text{atoms}}{\text{unit cell}} \cdot \dfrac{\text{volume}}{\text{atom}}}{\dfrac{\text{volume}}{\text{unit cell}}} = \frac{4 \cdot \frac{4}{3}\pi\left(\frac{\sqrt{2}a}{4}\right)^3}{a^3}$$

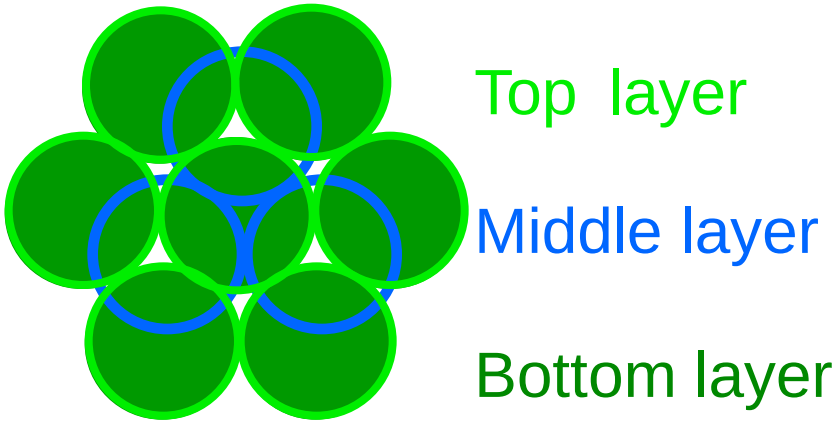
Hexagonal Close-Packed Structure (HCP)

- ABAB... Stacking Sequence
- 3D Projection



Adapted from Fig. 3.3(a), *Callister & Rethwisch 3e.*

- 2D Projection



- Coordination # = 12
- APF = 0.74
- *c*/*a* = 1.633

6 atoms/unit cell

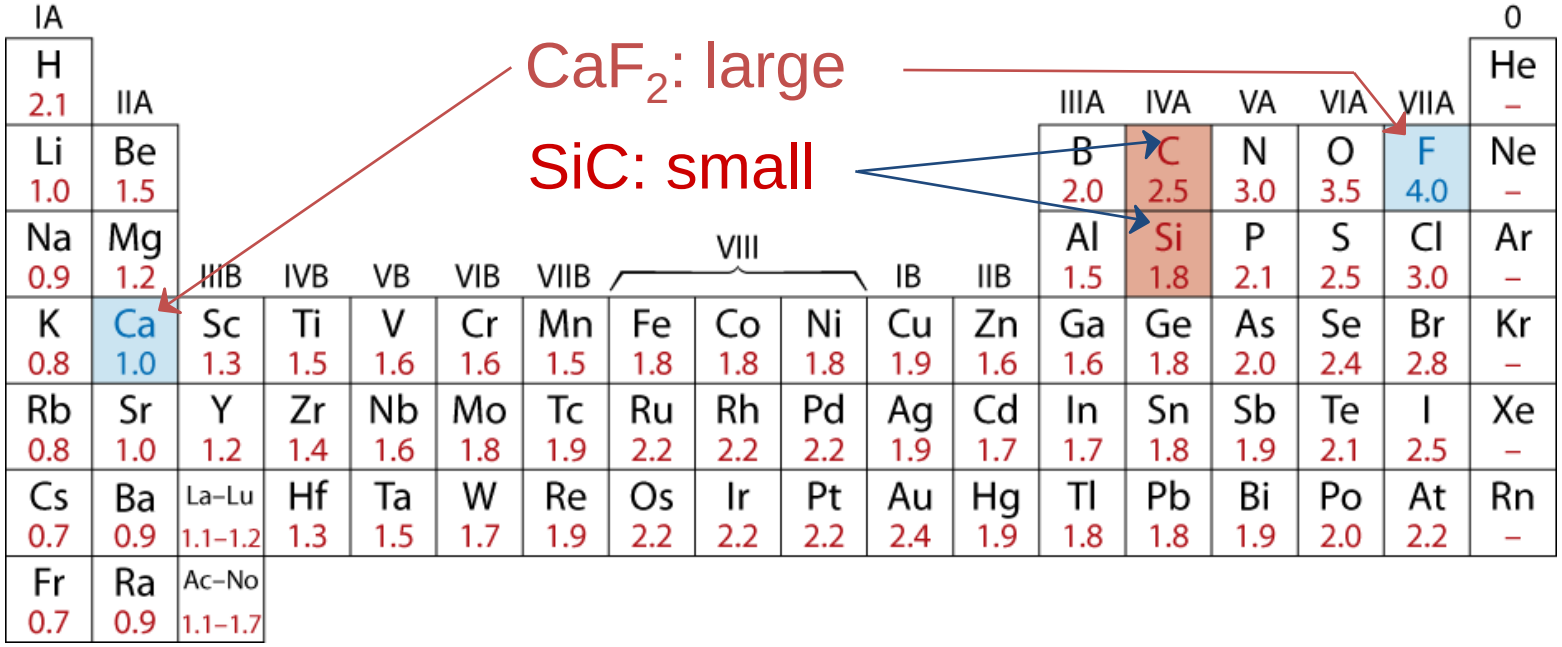
COMPARISON OF CRYSTAL STRUCTURES

Crystal structure	**packing factor**
• Simple Cubic (SC)	0.52
• Body Centered Cubic (BCC)	0.68
• Face Centered Cubic (FCC)	0.74
• Hexagonal Close Pack (HCP)	0.74

Ceramic Crystal Structures

Atomic Bonding in Ceramics

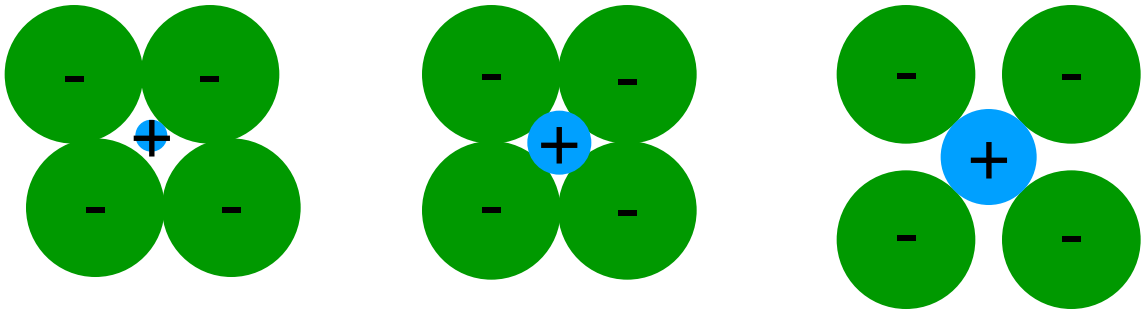
- Bonding:
  -- Can be ionic and/or covalent in character.
  -- % ionic character increases with difference in electronegativity of atoms.
- Degree of ionic character may be large or small:



Adapted from Fig. 2.7, *Callister & Rethwisch 3e.* (Fig. 2.7 is adapted from Linus Pauling, *The Nature of the Chemical Bond*, 3rd edition, Copyright 1939 and 1940, 3rd edition. Copyright 1960 by Cornell University.

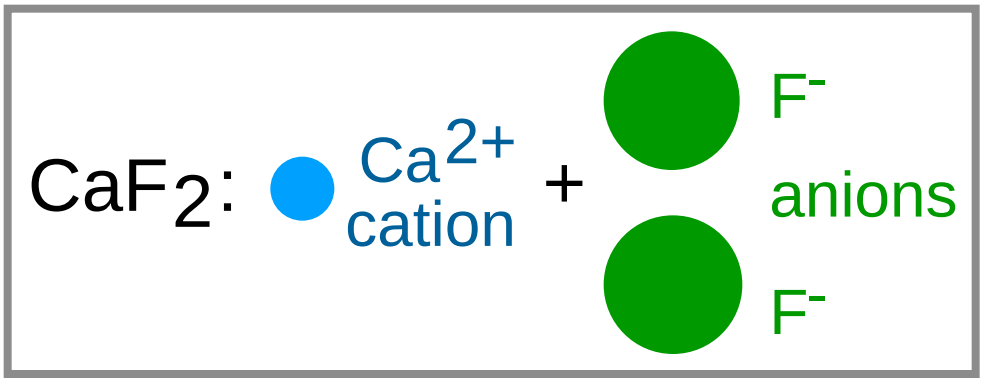
Factors that Determine Crystal Structure

1. Relative sizes of ions – Formation of stable structures:
   --maximize the # of oppositely charged ion neighbors.



Adapted from Fig. 3.4, *Callister & Rethwisch 3e.*

2. Maintenance of Charge Neutrality :
   --Net charge in ceramic should be zero.
   --Reflected in chemical formula:



$A_m X_p$

m, p values to achieve charge neutrality

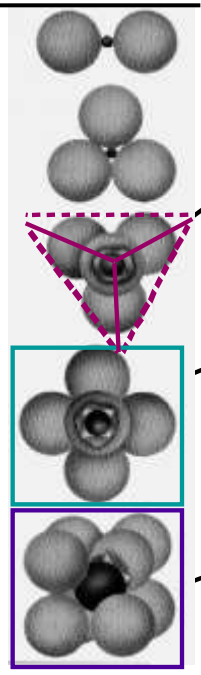
Coordination # and Ionic Radii

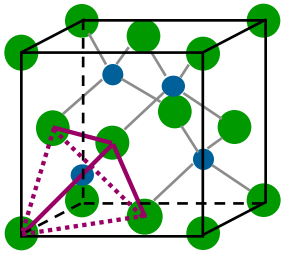
- Coordination # increases with $\frac{r_{cation}}{r_{anion}}$

To form a stable structure, how many anions can surround around a cation?

$\frac{r_{cation}}{r_{anion}}$	Coord #	
< 0.155	2	linear
0.155 - 0.225	3	triangular
0.225 - 0.414	4	tetrahedral
0.414 - 0.732	6	octahedral
0.732 - 1.0	8	cubic

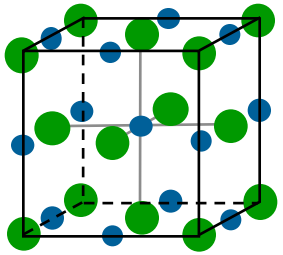
Adapted from Table 3.3, *Callister & Rethwisch 3e.*





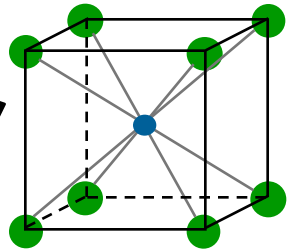
ZnS (zinc blende)

Adapted from Fig. 3.7, *Callister & Rethwisch 3e.*



NaCl (sodium chloride)

Adapted from Fig. 3.5, *Callister & Rethwisch 3e.*



CsCl (cesium chloride)

Adapted from Fig. 3.6, *Callister & Rethwisch 3e.*

Example Problem: Predicting the Crystal Structure of FeO

- On the basis of ionic radii, what crystal structure would you predict for FeO?

Cation	Ionic radius (nm)
Al^{3+}	0.053
Fe^{2+}	0.077
Fe^{3+}	0.069
Ca^{2+}	0.100

Anion	
O^{2-}	0.140
Cl^{-}	0.181
F^{-}	0.133

Data from Table 3.4,
Callister & Rethwisch 3e.

- Answer:

$$\frac{r_{cation}}{r_{anion}} = \frac{0.077}{0.140}$$

$$= 0.550$$

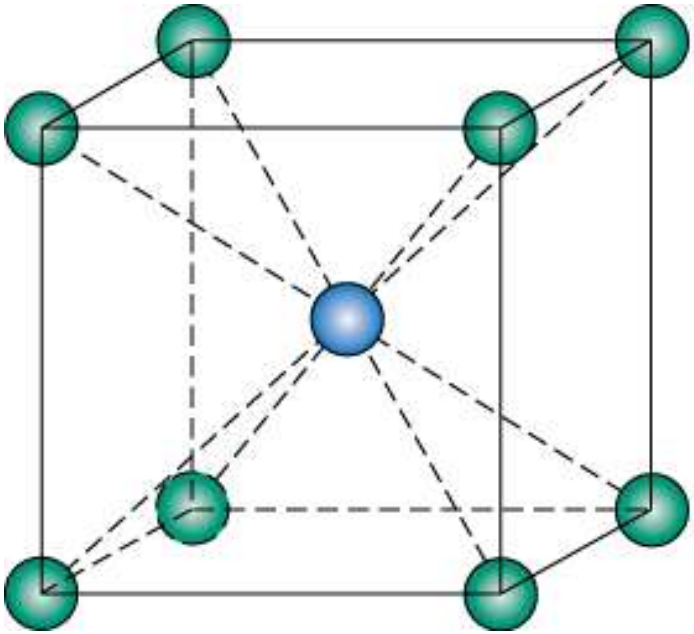
based on this ratio,
-- coord # = 6 because

$$0.414 < 0.550 < 0.732$$

-- crystal structure is NaCl

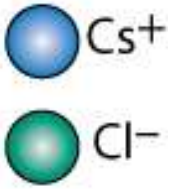
AX Crystal Structures

- Equal No. of cations and anions
- AX–Type Crystal Structures include NaCl, CsCl, and zinc blende



Adapted from Fig. 3.6, *Callister & Rethwisch 3e.*

Cesium Chloride structure:

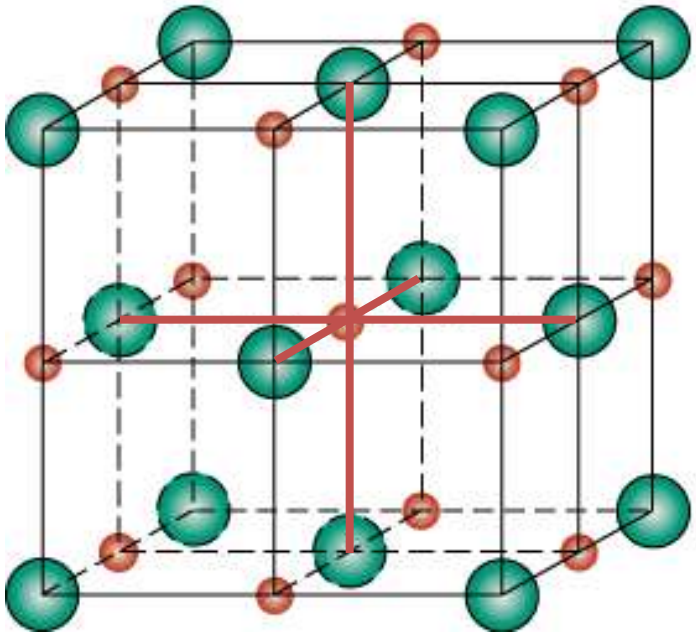


$$\frac{r_{Cs^+}}{r_{Cl^-}} = \frac{0.170}{0.181} = 0.939$$

$\therefore$ Since 0.732 < 0.939 < 1.0, cubic sites preferred

So each Cs^+ has 8 neighbor Cl^-

Rock Salt Structure



Adapted from Fig. 3.5,
Callister & Rethwisch 3e.

Na^+ $r_{Na} = 0.102$ nm

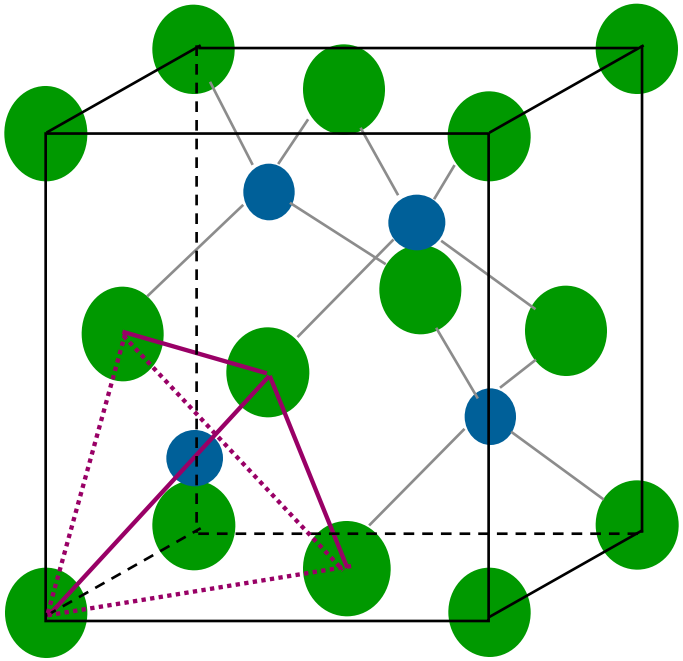
Cl^- $r_{Cl} = 0.181$ nm

$r_{Na}/r_{Cl} = 0.564$

$\therefore$ Since $0.414 < 0.564 < 0.732$,
Octahedral sites preferred

So each Na^+ has 6 neighbor Cl^-

Zinc Blende (ZnS) Structure



Adapted from Fig. 3.7,
Callister & Rethwisch 3e.

Zn^{2+}

S^{2-}

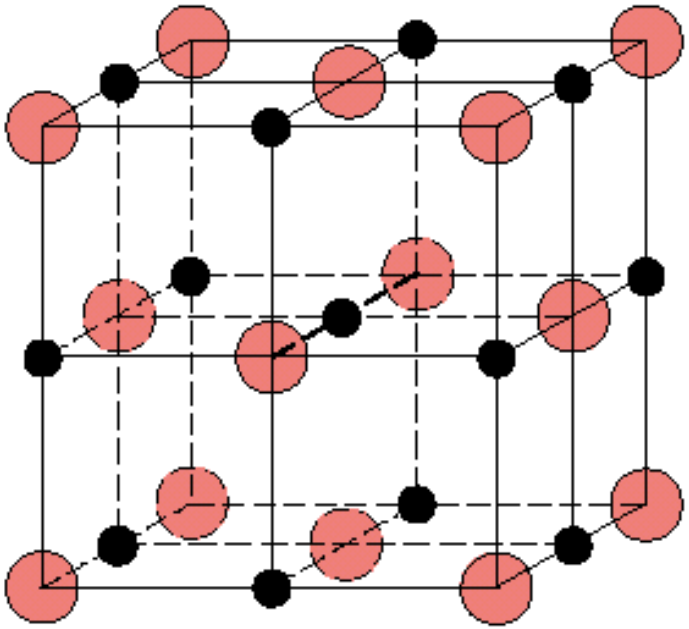
$r_{Zn}/r_S = 0.074/0.184 = 0.402$

$\therefore$ Since $0.225 < 0.402 < 0.414$, tetrahedral sites preferred

So each Zn^{++} has 4 neighbor S^{--}

MgO and FeO

MgO and FeO also have the NaCl structure



Adapted from Fig. 3.5,
Callister & Rethwisch 3e.

O^{2-} $r_O = 0.140$ nm

Mg^{2+} $r_{Mg} = 0.072$ nm

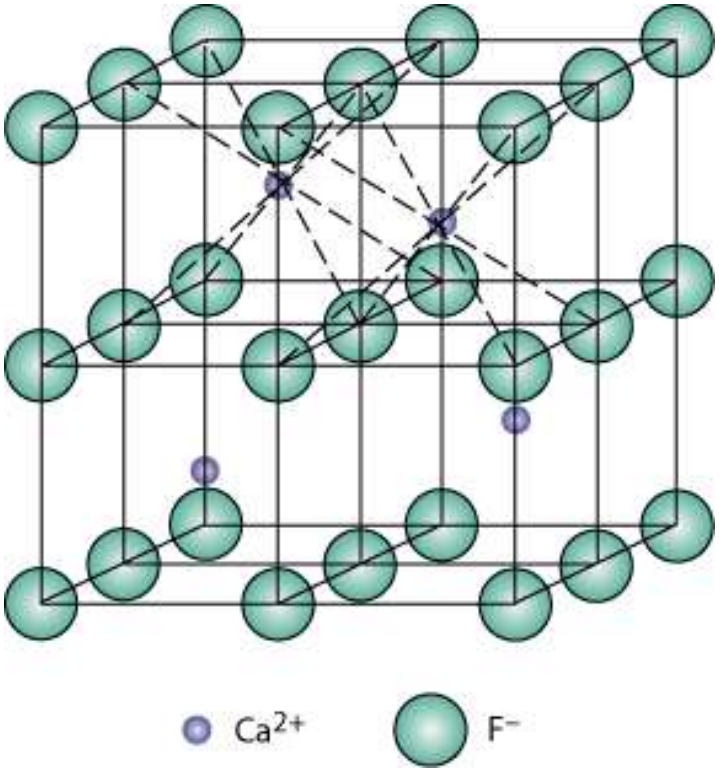
$r_{Mg}/r_O = 0.514$

$\therefore$ cations prefer octahedral sites

So each Mg^{2+} (or Fe^{2+}) has 6 neighbor oxygen atoms

A_mX_p Crystal Structures

m and/or p ≠ 1, e.g AX_2



Adapted from Fig. 3.8, *Callister & Rethwisch 3e.*

- Calcium Fluorite (CaF_2)
- Cations in cubic sites

- UO_2, ThO_2, ZrO_2, CeO_2

- Antifluorite structure – positions of cations and anions reversed

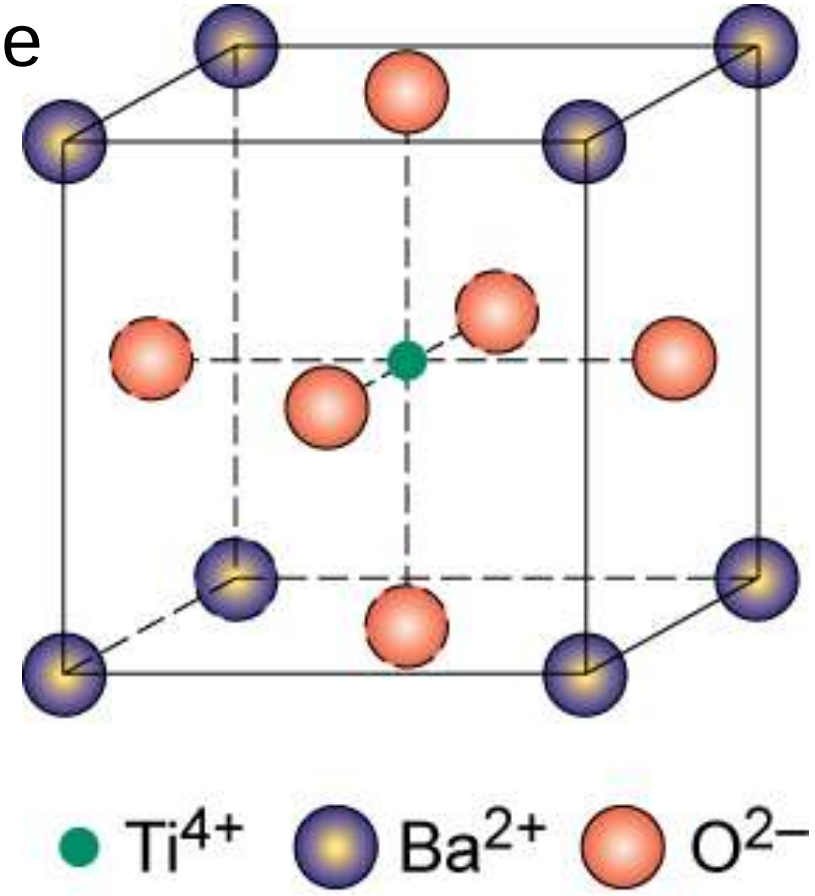
Fluorite structure

ABX_3 Crystal Structures

- Perovskite structure

Ex: complex oxide

$BaTiO_3$



Adapted from Fig. 3.9,
Callister & Rethwisch 3e.

Densities of Material Classes

In general

$\rho_{metals} > \rho_{ceramics} > \rho_{polymers}$

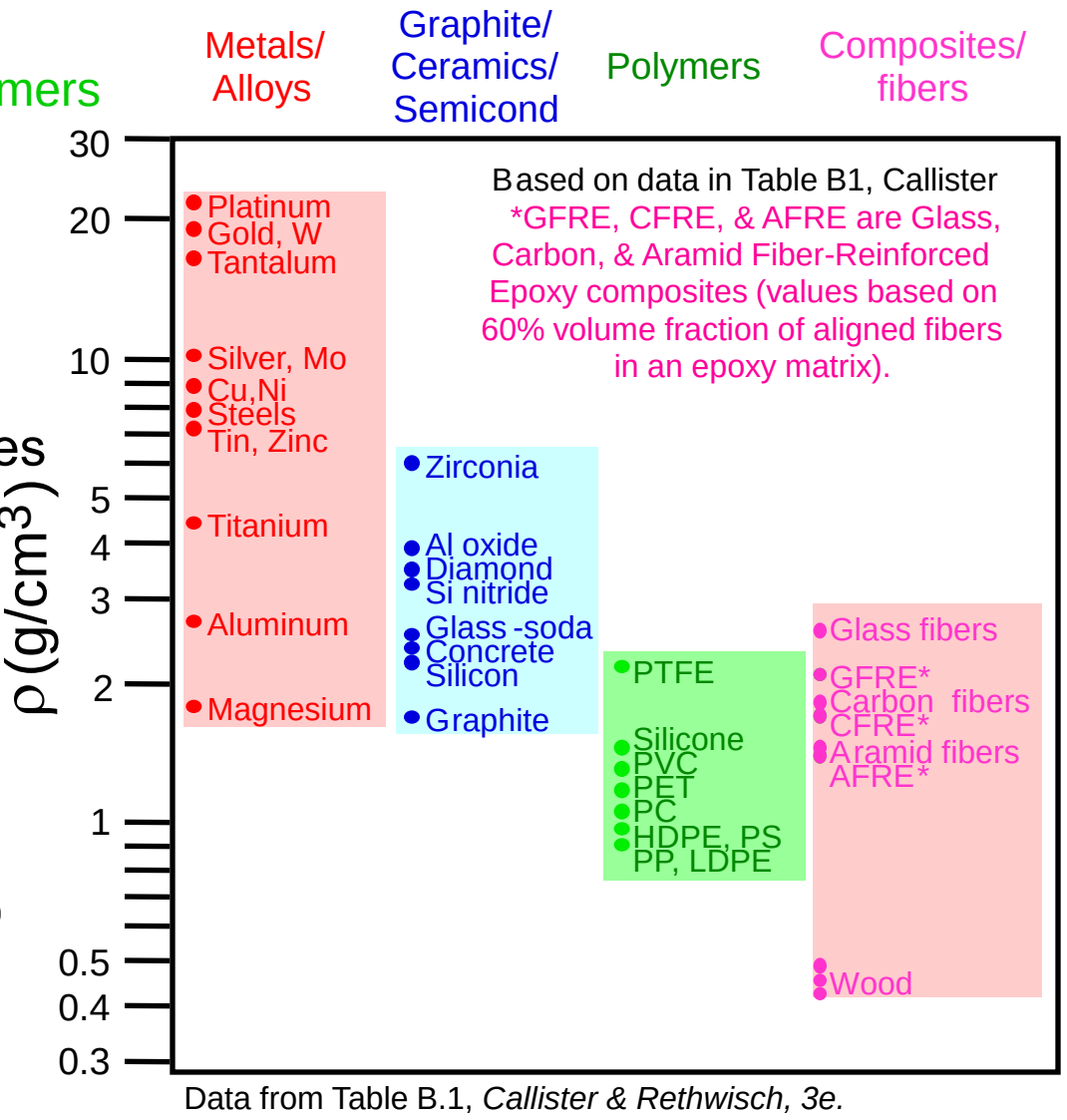
Why?

Metals have...
- close-packing (metallic bonding)
- often large atomic masses

Ceramics have...
- less dense packing
- often lighter elements

Polymers have...
- low packing density (often amorphous)
- lighter elements (C,H,O)

Composites have...
- intermediate values



Data from Table B.1, *Callister & Rethwisch, 3e.*

Crystals as Building Blocks

- *Some* engineering applications require single crystals:
  -- diamond single crystals for abrasives

(Courtesy Martin Deakins, GE Superabrasives, Worthington, OH. Used with permission.)

-- turbine blades

Fig. 9.40(c), *Callister & Rethwisch 3e.* (Fig. 9.40(c) courtesy of Pratt and Whitney).

- Properties of crystalline materials often related to crystal structure.

  -- Ex: Quartz fractures more easily along some crystal planes than others.

(Courtesy P.M. Anderson)

Polycrystals

- *Most* engineering materials are polycrystals.

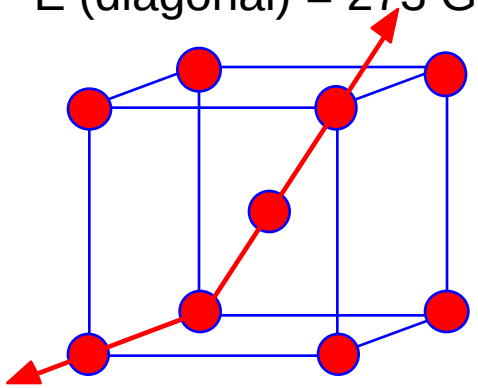
Adapted from Fig. K, color inset pages of *Callister 5e*.
(Fig. K is courtesy of Paul E. Danielson, Teledyne Wah Chang Albany)

- Nb-Hf-W plate with an electron beam weld.
- Each "grain" is a single crystal.
- If grains are randomly oriented,
  overall component properties are not directional.
- Grain sizes typ. range from 1 nm to 2 cm
  (i.e., from a few to millions of atomic layers).

Single vs Polycrystals

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

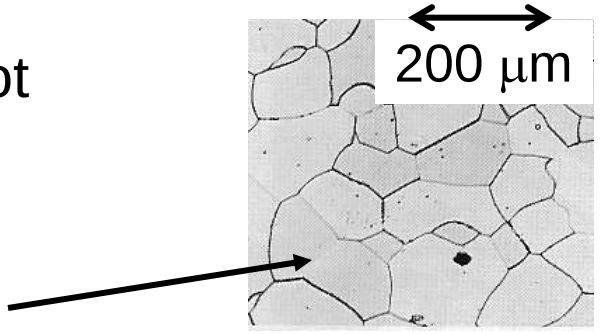
E (diagonal) = 273 GPa

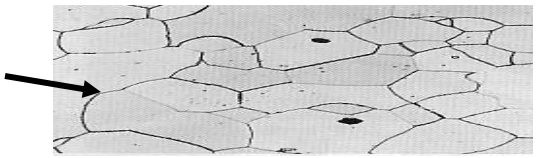


E (edge) = 125 GPa

Data from Table 3.7, *Callister & Rethwisch 3e*. (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.
    ($E_{poly\ iron}$ = 210 GPa)
  - -If grains are textured, anisotropic.





Adapted from Fig. 5.19(b), *Callister & Rethwisch 3e*. (Fig. 5.19(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].)

Polymorphism

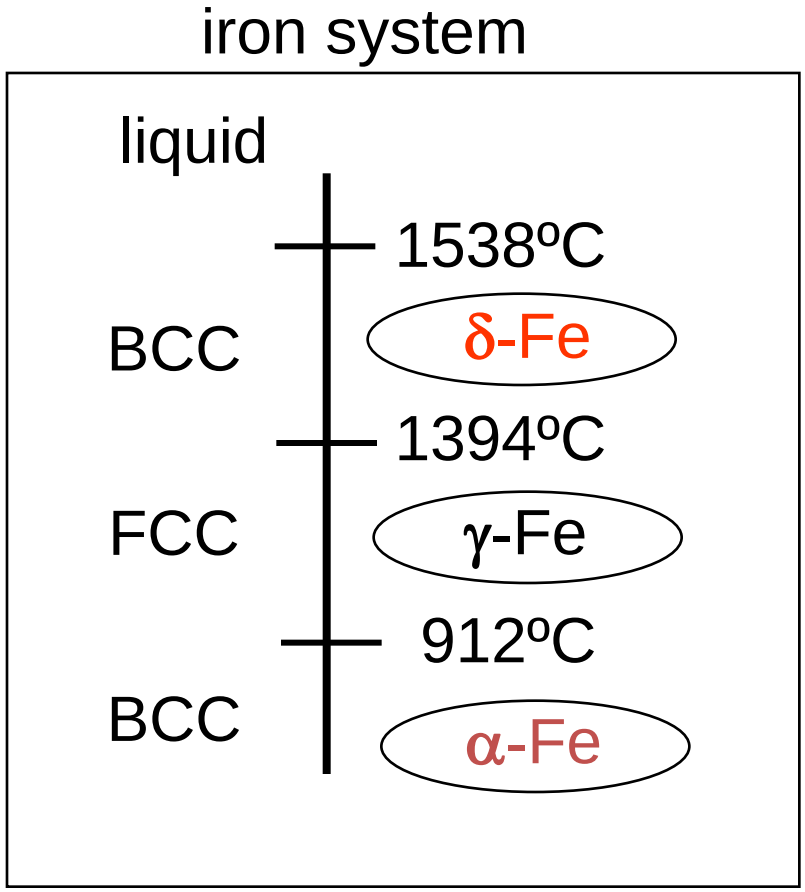
- Two or more distinct crystal structures for the same material (allotropy/polymorphism)

titanium

α, β-Ti

carbon

diamond, graphite



Crystal Systems

Unit cell: smallest repetitive volume which contains the complete lattice pattern of a crystal.

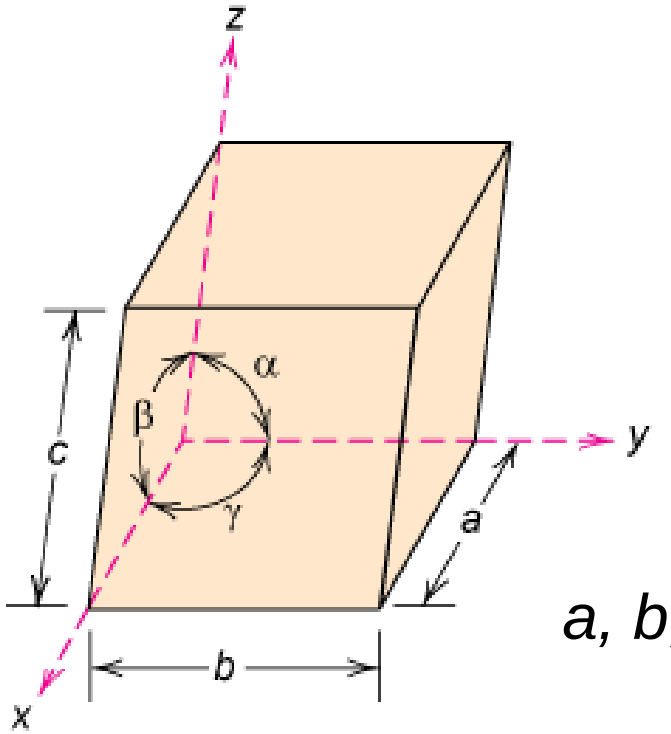


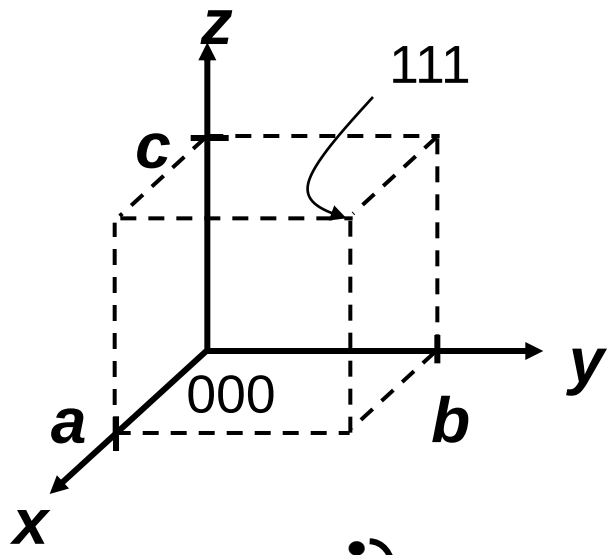
Fig. 3.20, *Callister & Rethwisch 3e.*

7 crystal systems

14 crystal lattices

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

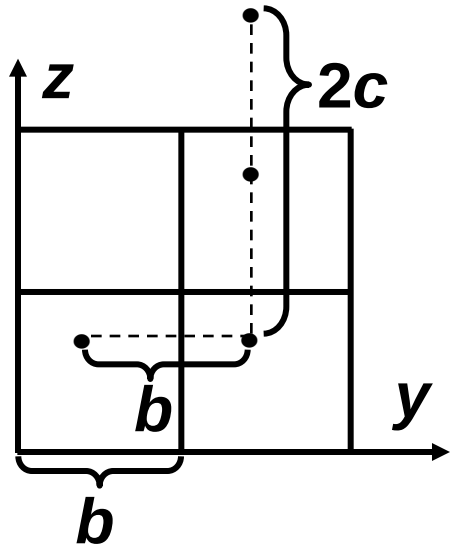
Point Coordinates



Point coordinates for unit cell center are

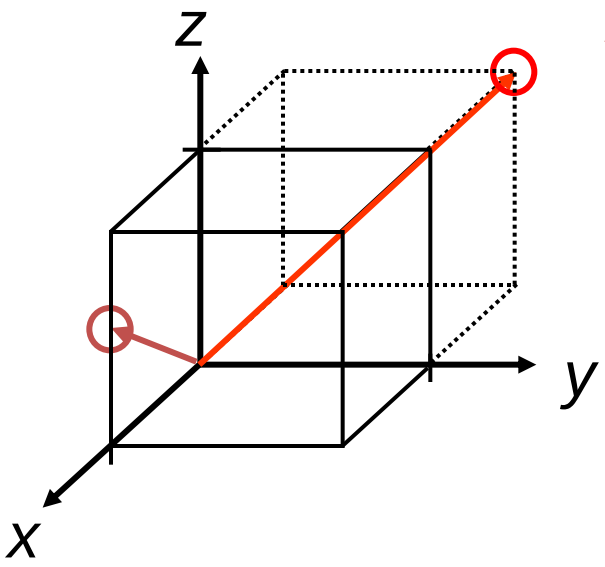
$a/2, b/2, c/2$ ½½½

Point coordinates for unit cell corner are 111



Translation: integer multiple of lattice constants → identical position in another unit cell

Crystallographic Directions



Algorithm

1. Vector repositioned (if necessary) to pass through origin.
2. Read off projections in terms of unit cell dimensions *a*, *b*, and *c*
3. Adjust to smallest integer values
4. Enclose in square brackets, no commas

[*uvw*]

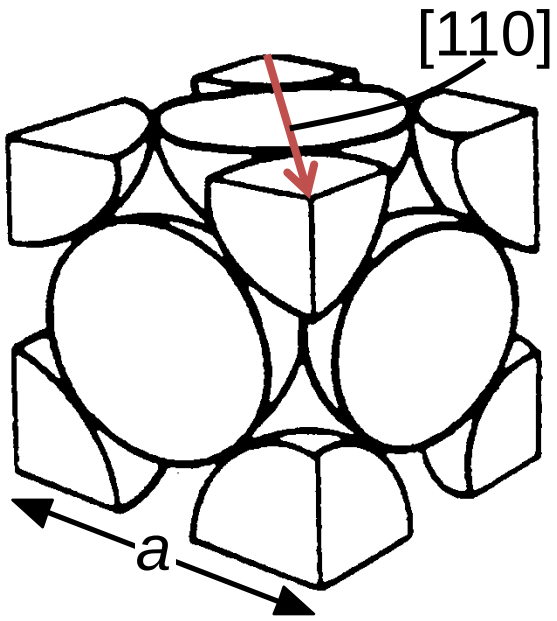
ex: 1, 0, ½ => 2, 0, 1 => [201]

-1, 1, 1 => $[\bar{1}11]$ where overbar represents a negative index

families of directions <*uvw*>

Linear Density

- Linear Density of Atoms ≡ LD = $\dfrac{\text{Number of atoms}}{\text{Unit length of direction vector}}$



ex: linear density of Al in [110] direction

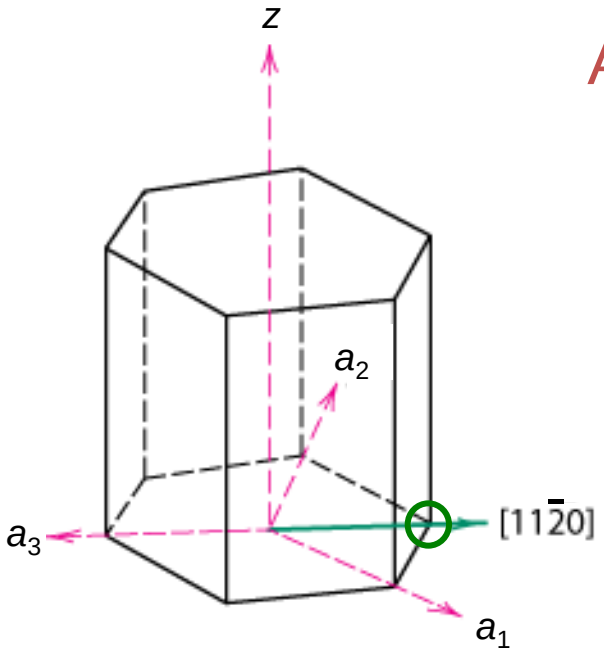
a = 0.405 nm

atoms → 2

$$LD = \frac{2}{\sqrt{2}a} = 3.5\ \text{nm}^{-1}$$

length → $\sqrt{2}a$

HCP Crystallographic Directions



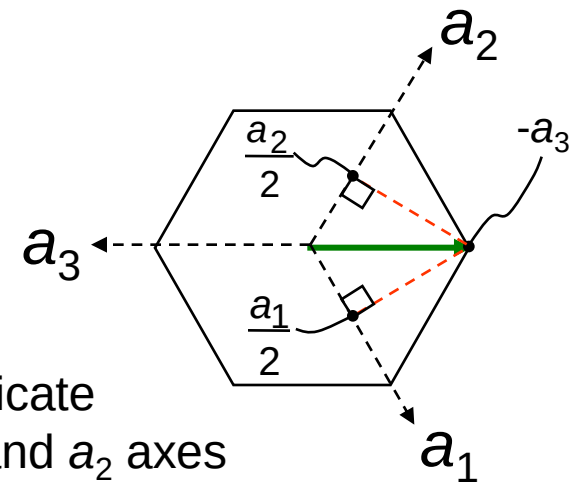
Adapted from Fig. 3.24(a), *Callister & Rethwisch 3e.*

Algorithm

1. Vector repositioned (if necessary) to pass through origin.
2. Read off projections in terms of unit cell dimensions a_1, a_2, a_3, or c
3. Adjust to smallest integer values
4. Enclose in square brackets, no commas

[*uvtw*]

ex: ½, ½, -1, 0 => $[11\bar{2}0]$



dashed red lines indicate projections onto a_1 and a_2 axes

HCP Crystallographic Directions

- Hexagonal Crystals
  - 4 parameter Miller-Bravais lattice coordinates are related to the direction indices (i.e., *u'v'w'*) as follows.

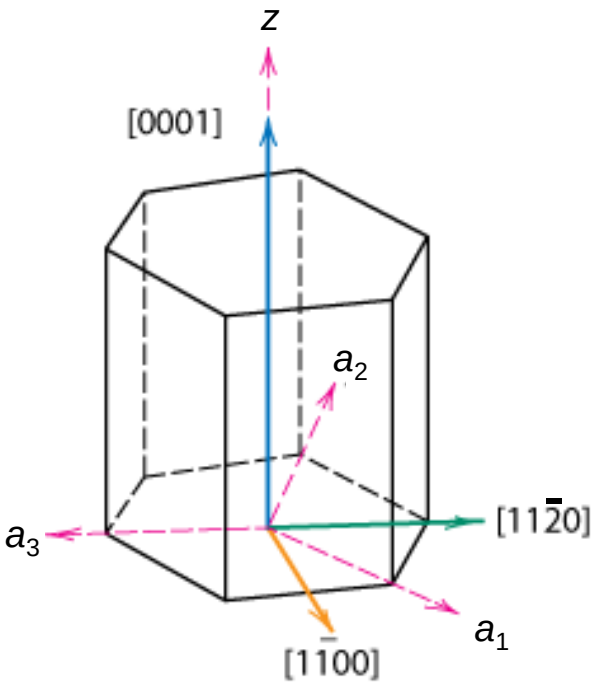


Fig. 3.24(a), *Callister & Rethwisch 3e.*

$$[u'v'w'] \rightarrow [uvtw]$$

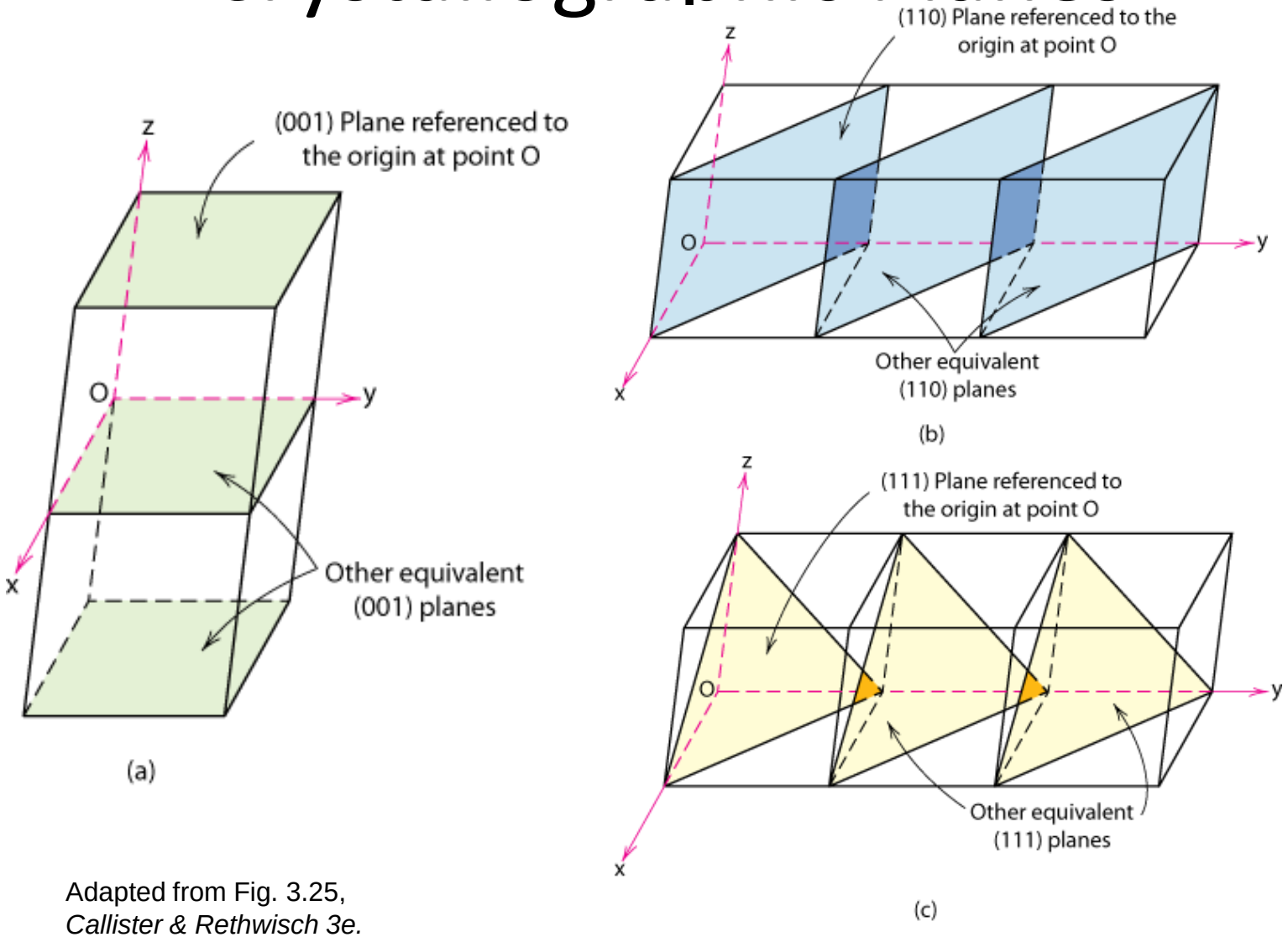
$$u = \frac{1}{3}(2u' - v')$$

$$v = \frac{1}{3}(2v' - u')$$

$$t = -(u + v)$$

$$w = w'$$

Crystallographic Planes



Adapted from Fig. 3.25,
Callister & Rethwisch 3e.

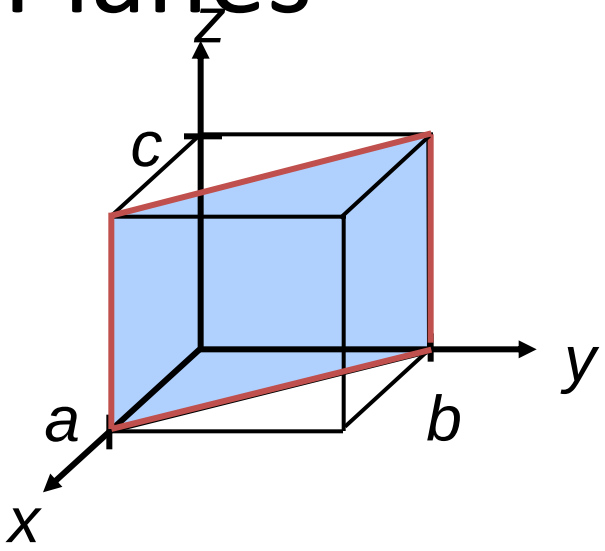
Crystallographic Planes

- Miller Indices: Reciprocals of the (three) axial intercepts for a plane, cleared of fractions & common multiples. All parallel planes have same Miller indices.

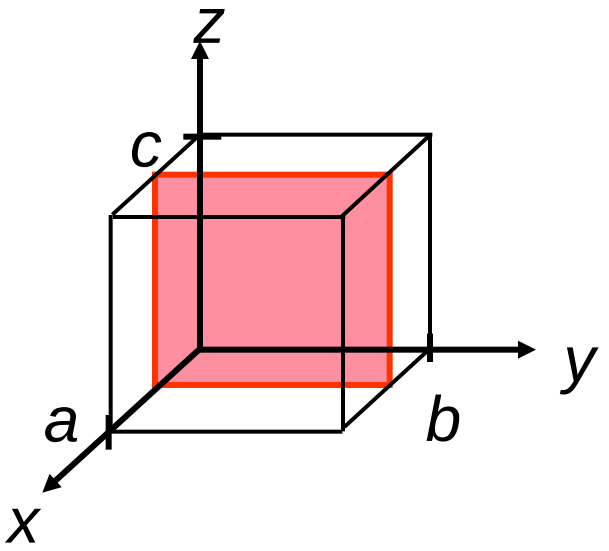
- Algorithm
  1. Read off intercepts of plane with axes in terms of *a*, *b*, *c*
  2. Take reciprocals of intercepts
  3. Reduce to smallest integer values
  4. Enclose in parentheses, no commas i.e., (*hkl*)

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)		

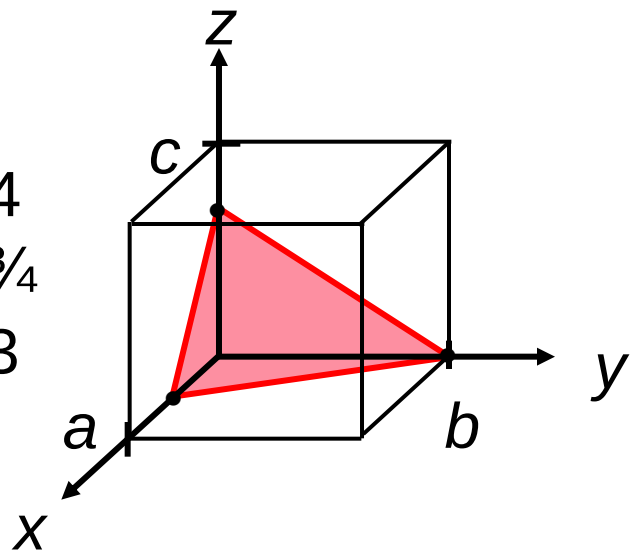


example		*a*	*b*	*c*
1.	Intercepts	1/2	∞	∞
2.	Reciprocals	1/½	1/∞	1/∞
		2	0	0
3.	Reduction	2	0	0
4.	Miller Indices	(100)		



Crystallographic Planes

example		*a*	*b*	*c*
1.	Intercepts	1/2	1	3/4
2.	Reciprocals	1/½	1/1	1/¾
		2	1	4/3
3.	Reduction	6	3	4
4.	Miller Indices	(634)		



Family of Planes {*hkl*}

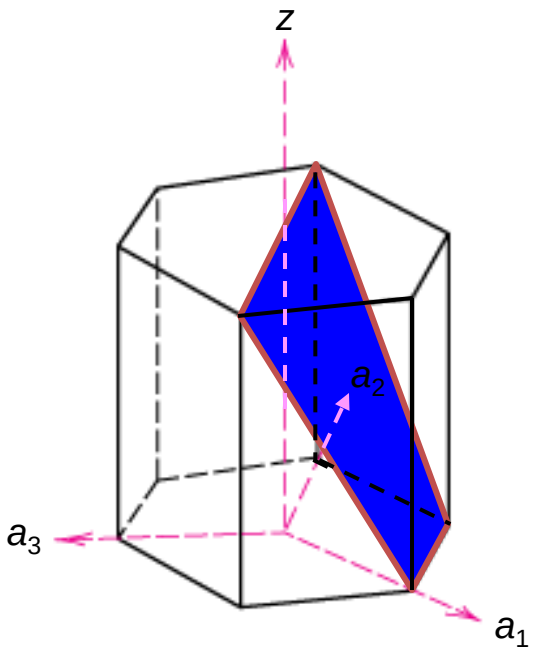
Ex: {100} = (100), (010), (001), ($\bar{1}$00), (0$\bar{1}$0), (00$\bar{1}$)

Crystallographic Planes (HCP)

- In hexagonal unit cells the same idea is used

example	a_1	a_2	a_3	c
1. Intercepts	1	∞	-1	1
2. Reciprocals	1	$1/\infty$	-1	1
	1	0	-1	1
3. Reduction	1	0	-1	1

4. Miller-Bravais Indices $(10\bar{1}1)$



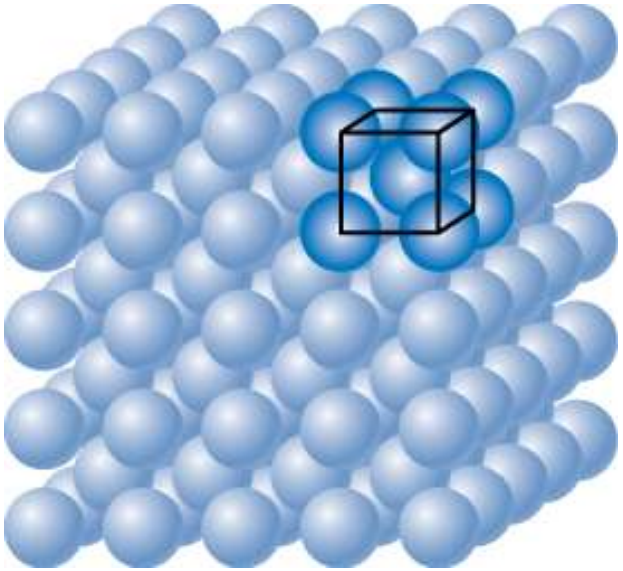
Adapted from Fig. 3.24(b), *Callister & Rethwisch 3e.*

Crystallographic Planes

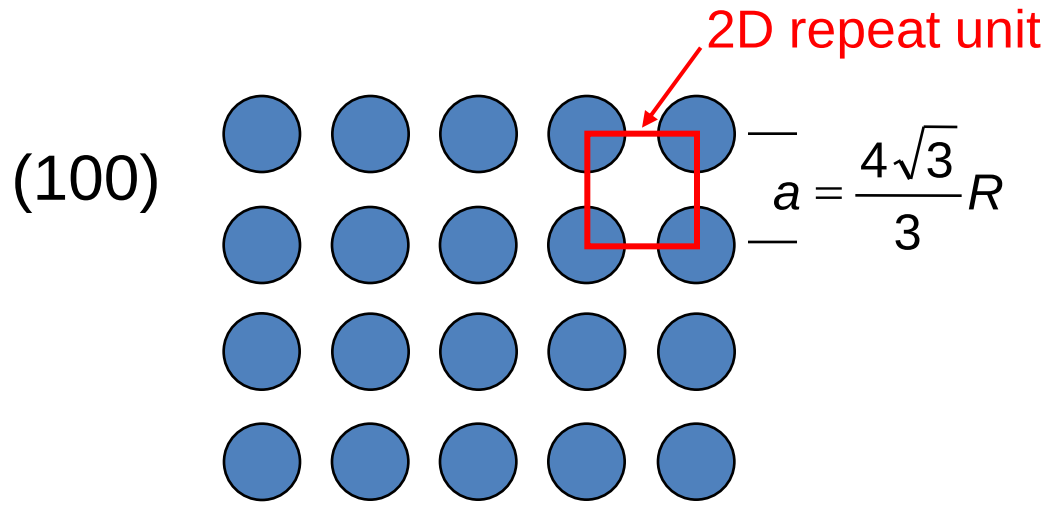
- We want to examine the atomic packing of crystallographic planes
- Iron foil can be used as a catalyst. The atomic packing of the exposed planes is important.
  a) Draw (100) and (111) crystallographic planes for Fe.
  b) Calculate the planar density for each of these planes.

Planar Density of (100) Iron

Solution: At T < 912°C iron has the BCC structure.



Adapted from Fig. 3.2(c), *Callister & Rethwisch 3e.*

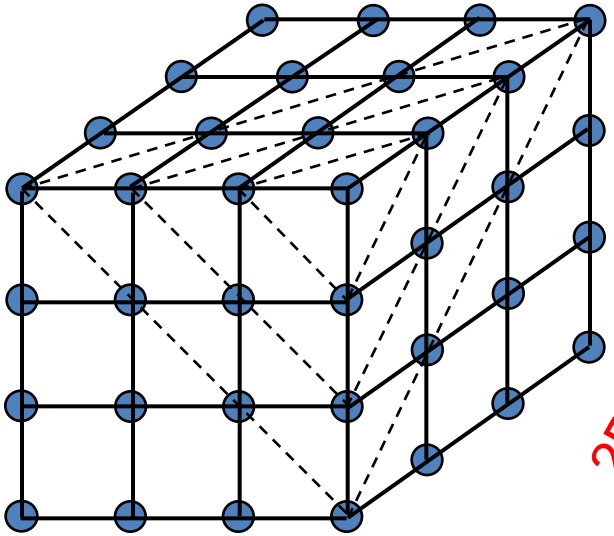


Radius of iron R = 0.1241 nm

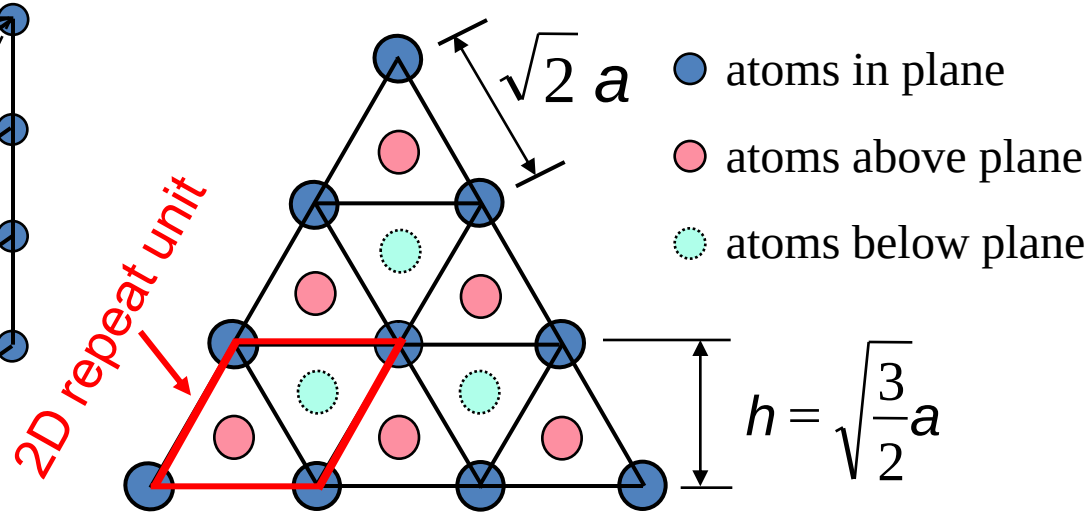
$$\text{Planar Density} = \frac{\dfrac{\text{atoms}}{\text{2D repeat unit}}}{\dfrac{\text{area}}{\text{2D repeat unit}}} = \frac{1}{a^2} = \frac{1}{\left(\frac{4\sqrt{3}}{3}R\right)^2} = 12.1\,\frac{\text{atoms}}{\text{nm}^2} = 1.2 \times 10^{19}\,\frac{\text{atoms}}{\text{m}^2}$$

Planar Density of (111) Iron

Solution (cont): (111) plane



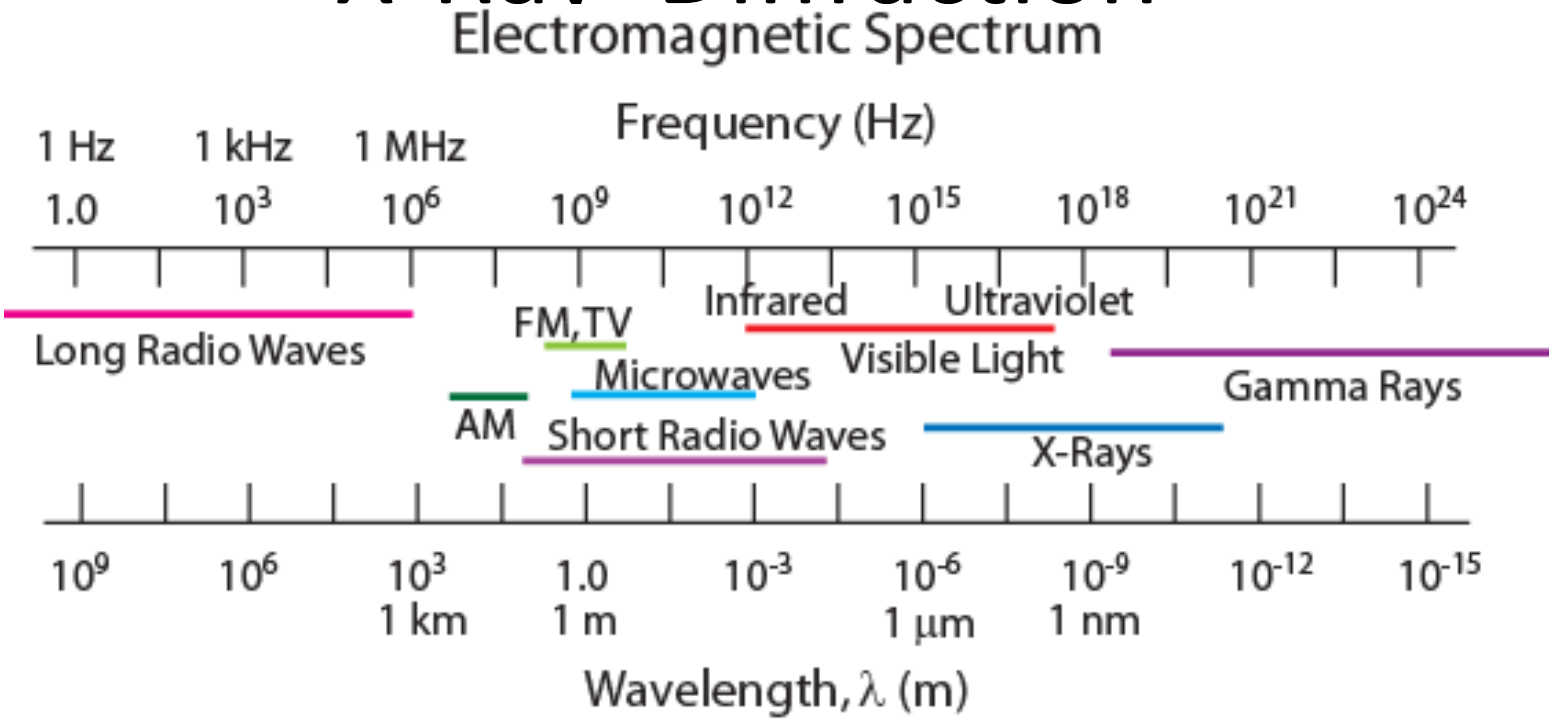
1 atom in plane/ unit surface cell



$$\text{area} = \sqrt{2}\,ah = \sqrt{3}\,a^2 = \sqrt{3}\left(\frac{4\sqrt{3}}{3}R\right)^2 = \frac{16\sqrt{3}}{3}R^2$$

$$\text{Planar Density} = \frac{\dfrac{\text{atoms}}{\text{2D repeat unit}}}{\dfrac{\text{area}}{\text{2D repeat unit}}} = \frac{1}{\frac{16\sqrt{3}}{3}R^2} = 7.0\,\frac{\text{atoms}}{\text{nm}^2} = 0.70 \times 10^{19}\,\frac{\text{atoms}}{\text{m}^2}$$

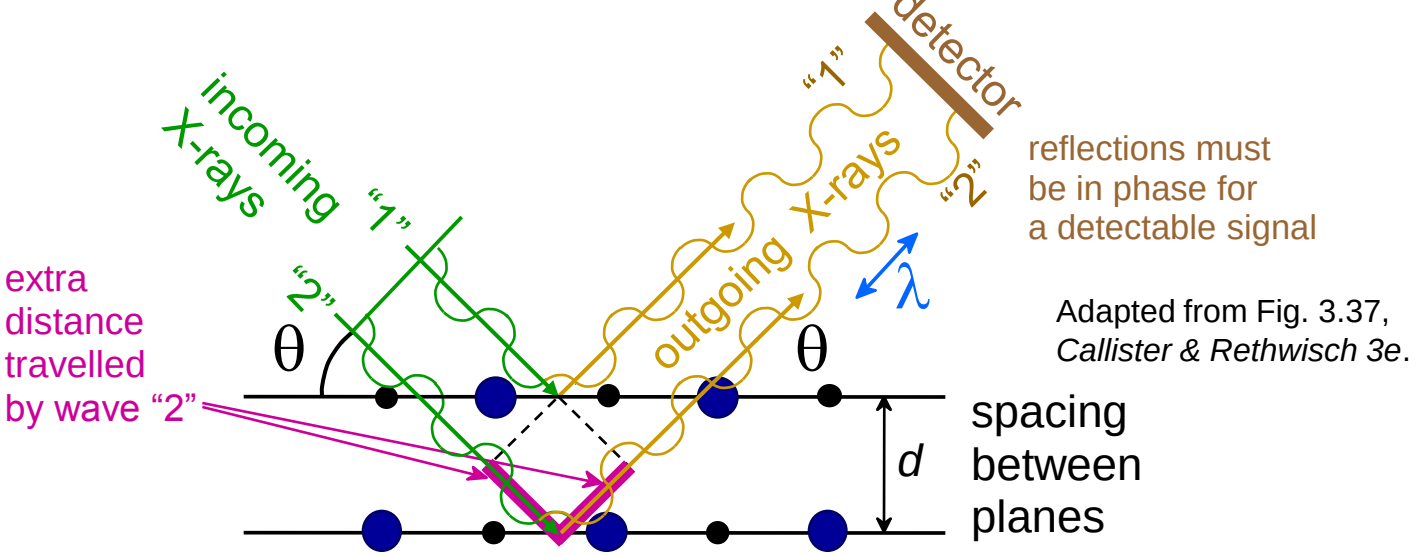
X-Rav Diffraction



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

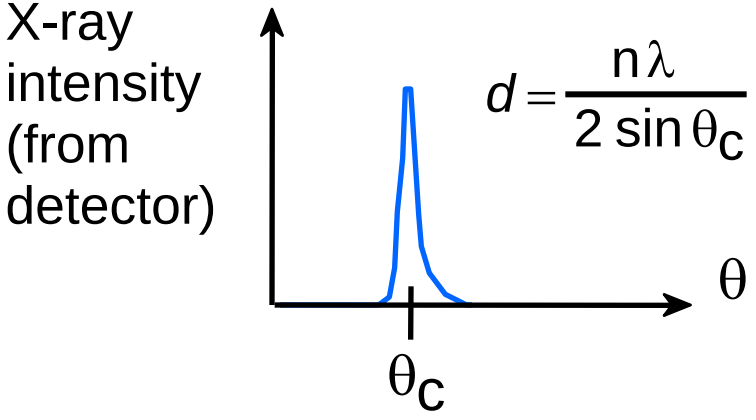
X-Rays to Determine Crystal Structure

- Incoming X-rays diffract from crystal planes.

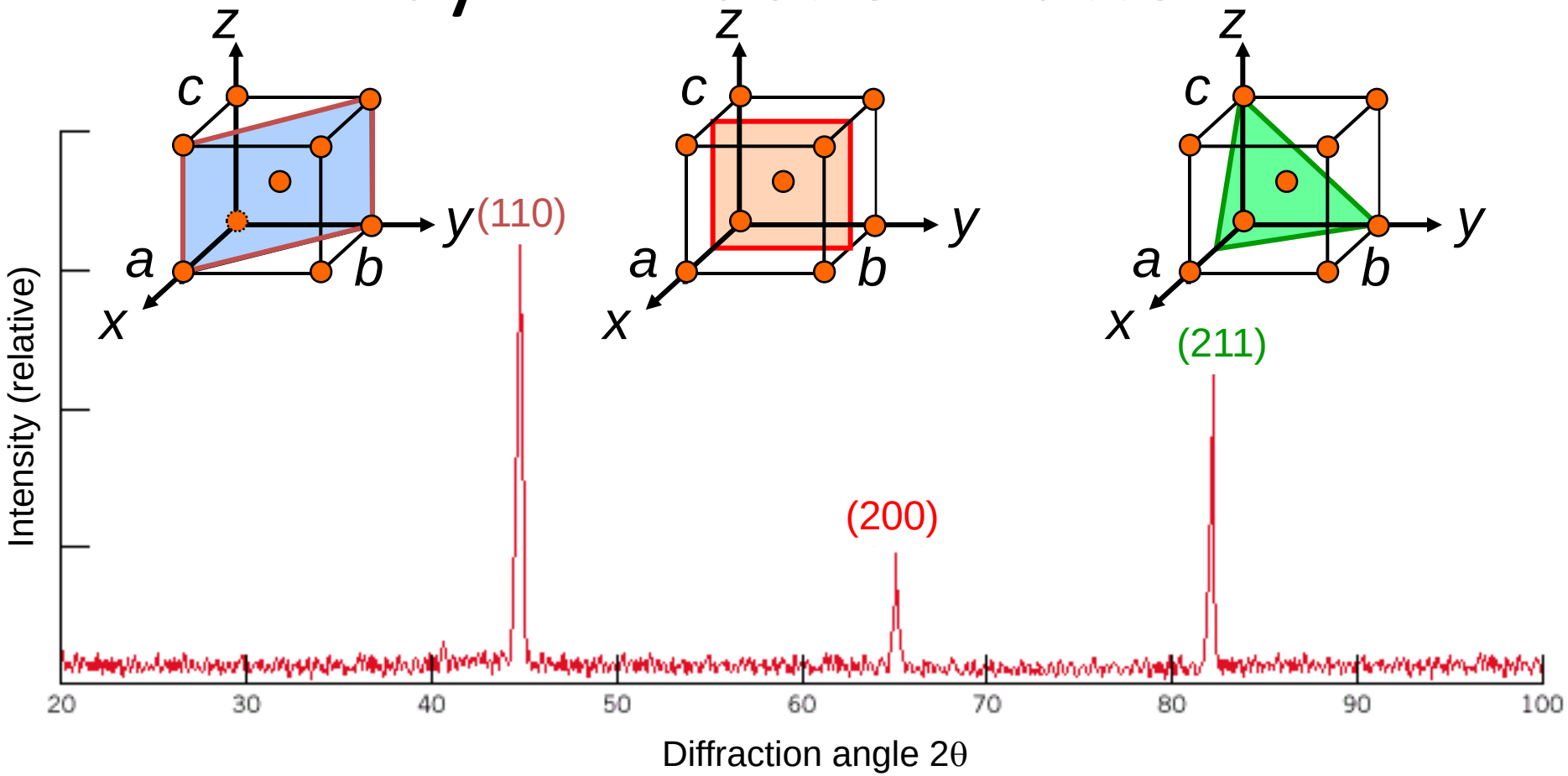


Adapted from Fig. 3.37, *Callister & Rethwisch 3e*.

Measurement of critical angle, θ_c, allows computation of planar spacing, *d*.



X-Ray Diffraction Pattern



Diffraction pattern for polycrystalline α-iron (BCC)

Adapted from Fig. 3.20, *Callister 5e.*

SUMMARY

- Atoms may assemble into crystalline or amorphous structures.
- Common metallic crystal structures are FCC, BCC, and HCP. Coordination number and atomic packing factor are the same for both FCC and HCP crystal structures.
- We can predict the density of a material, provided we know the atomic weight, atomic radius, and crystal geometry (e.g., FCC, BCC, HCP).
- Interatomic bonding in ceramics is ionic and/or covalent.
- Ceramic crystal structures are based on:
  -- maintaining charge neutrality
  -- cation-anion radii ratios.
- Crystallographic points, directions and planes are specified in terms of indexing schemes. Crystallographic directions and planes are related to atomic linear densities and planar densities.

SUMMARY

- Materials can be single crystals or polycrystalline. Material properties generally vary with single crystal orientation (i.e., they are anisotropic), but are generally non-directional (i.e., they are isotropic) in polycrystals with randomly oriented grains.
- Some materials can have more than one crystal structure. This is referred to as polymorphism (or allotropy).
- X-ray diffraction is used for crystal structure and interplanar spacing determinations.