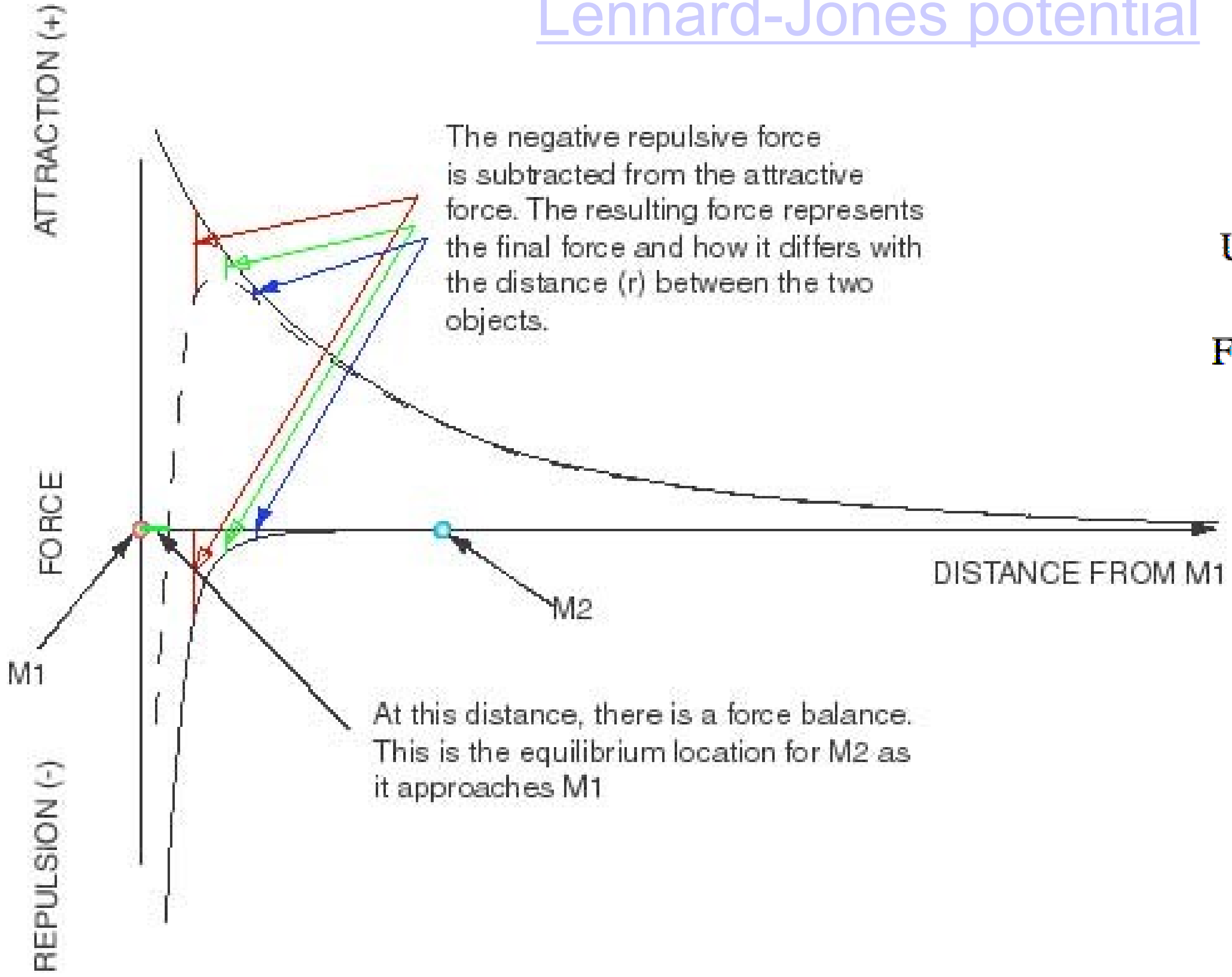
Chapter 3: The Structure of Crystalline Solids

ISSUES TO ADDRESS...

- How do atoms assemble into solid structures?
- How does the density of a material depend on its structure?
- When do material properties vary with the sample (i.e., part) orientation?

Lennard-Jones potential



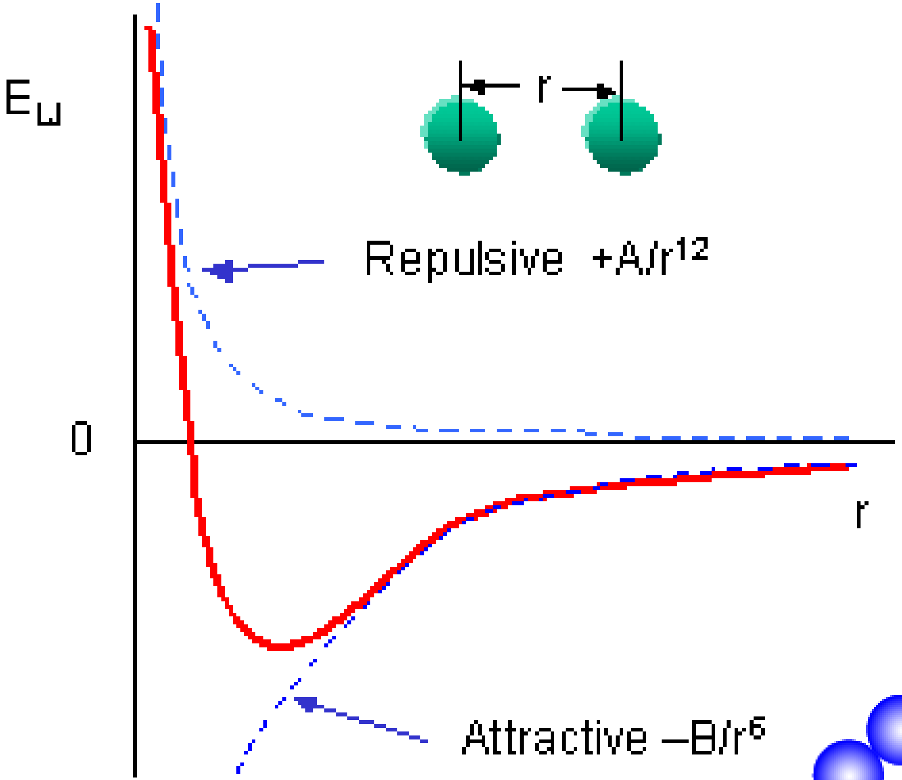
The negative repulsive force is subtracted from the attractive force. The resulting force represents the final force and how it differs with the distance (r) between the two objects.

At this distance, there is a force balance. This is the equilibrium location for M2 as it approaches M1

$$U(r) = -\frac{A}{r^n} + \frac{B}{r^m} \qquad (1)$$

$$F(r) = n\frac{A}{r^{n+1}} - m\frac{B}{r^{m+1}} \qquad (2)$$

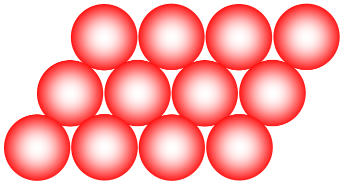
Energy and Packing

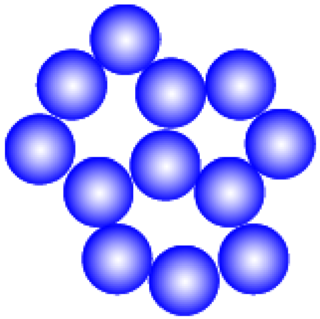


$$n\frac{A}{r_o^{n+1}} = m\frac{B}{r_o^{m+1}} \qquad \text{so}$$

$$\frac{r_o^{m+1}}{r_o^{n+1}} = r_o^{m-n} = \frac{mB}{nA} \qquad \text{and}$$

$$r_o = \sqrt[m-n]{\frac{mB}{nA}} \qquad (3)$$



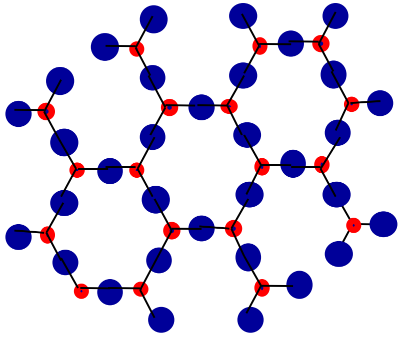


- Dense, ordered packing
- Non dense, random packing

Materials and Packing

Crystalline materials...

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



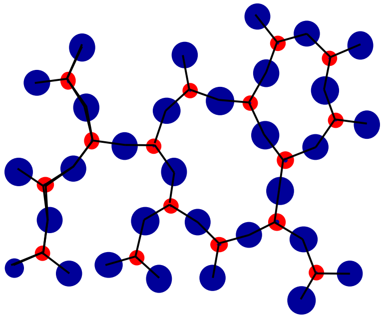
crystalline SiO_2

Adapted from Fig. 3.23(a), *Callister & Rethwisch 8e.*

● **Si** ● **Oxygen**

Noncrystalline materials...="Amorphous"

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



noncrystalline SiO_2

Adapted from Fig. 3.23(b), *Callister & Rethwisch 8e.*

پیوندهای اولیه: بین اتم ها و یون ها

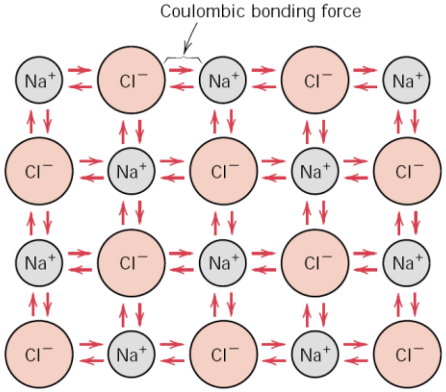
پیوندهای ثانویه: بین مولکول ها که ضعیفتر از پیوندهای اولیه هستند

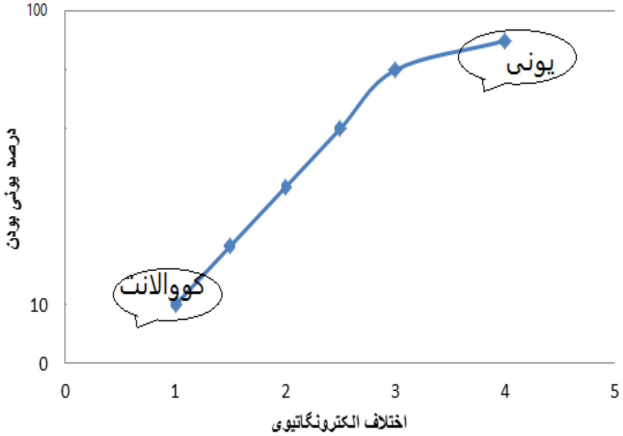
پیوندهای اولیه

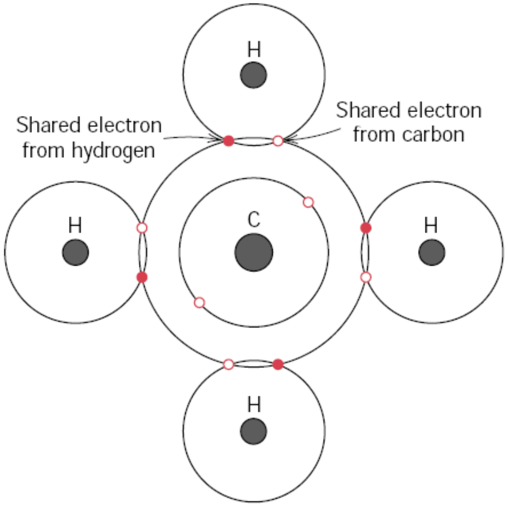
یونی: انتقال الکترون

کووالانسی یا کووالانت: بر اساس اشتراک الکترون هستند

فلزی



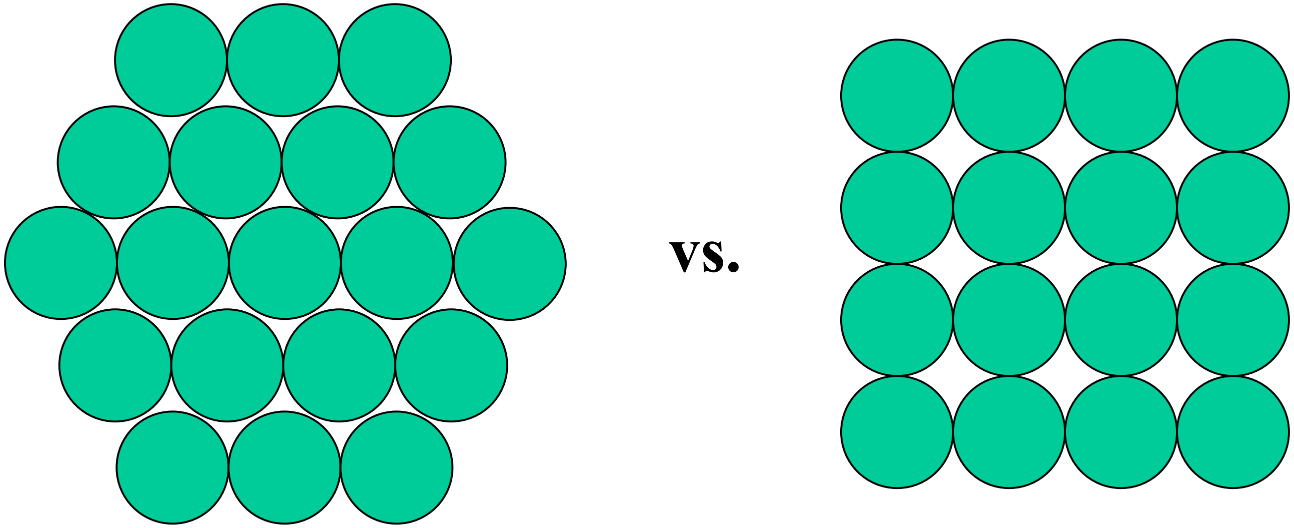




Metallic Crystal Structures

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

2-dimensions

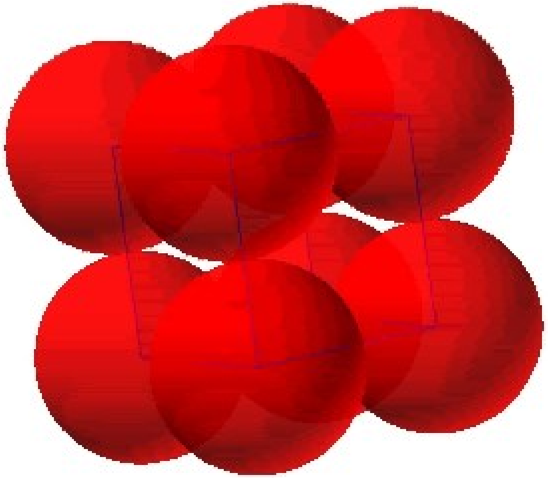


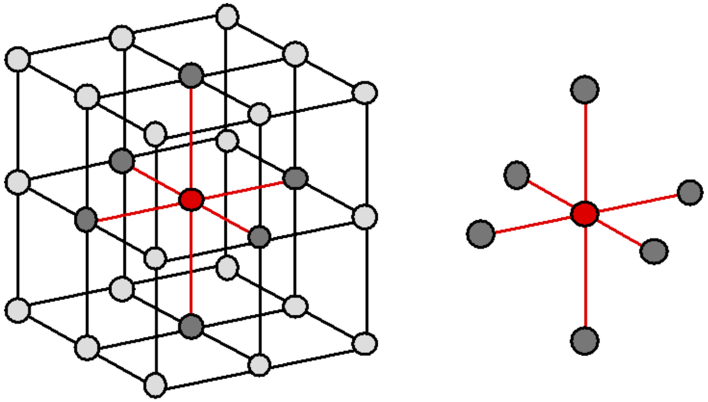
Now stack these 2-D layers to make 3-D structures

Simple Cubic Structure (SC)

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

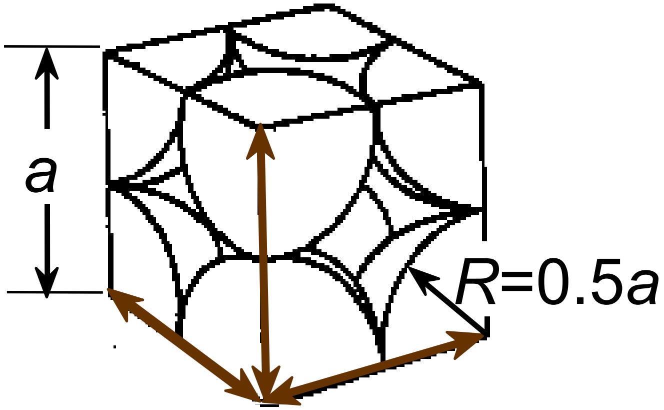
- Coordination N = 6





Atomic Packing Factor (APF)

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



contains 8 x 1/8 = 1 atom/unit cell

$$\text{APF} = \frac{\overset{\frac{\text{atoms}}{\text{unit cell}}}{1}\;\overset{\frac{\text{volume}}{\text{atom}}}{\frac{4}{3}\pi(0.5a)^3}}{\underset{\frac{\text{volume}}{\text{unit cell}}}{a^3}}$$

- APF SC = 0.52

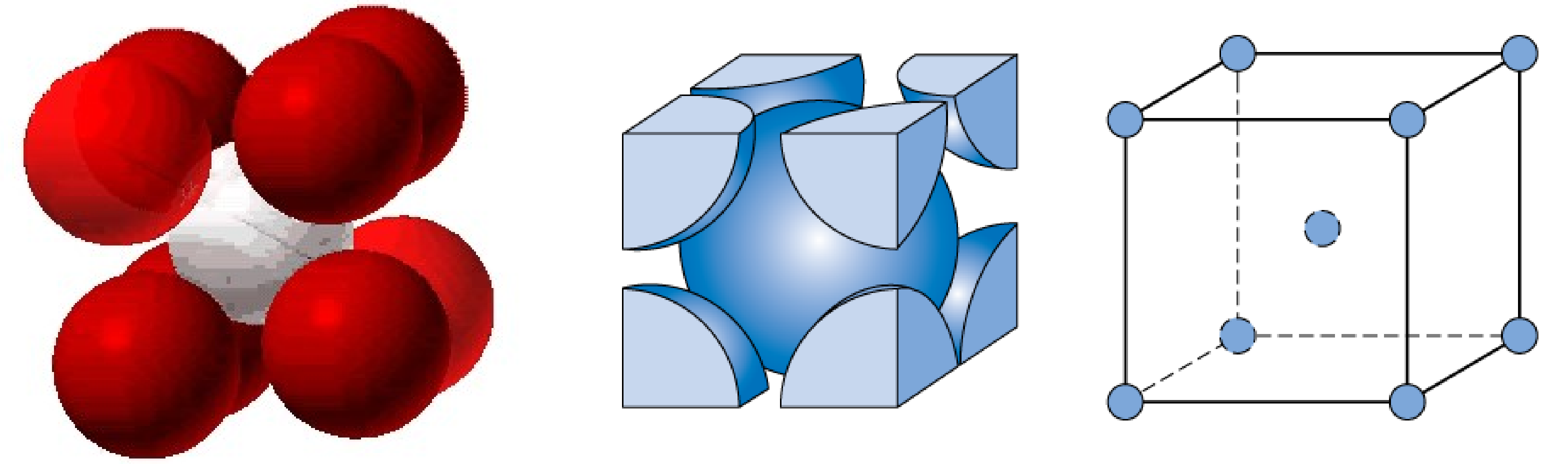
Body Centered Cubic Structure (BCC)

- Atoms touch each other along cube diagonals.

  Note: All atoms are identical

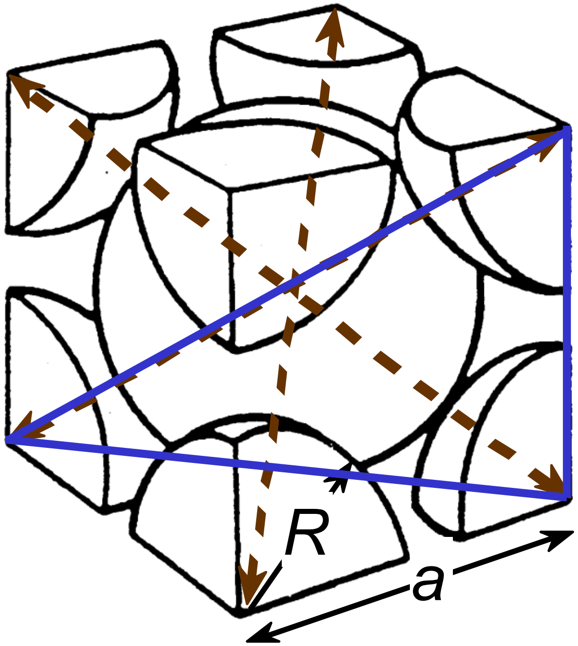
ex: Cr, W, Fe (α), Tantalum, Molybdenum

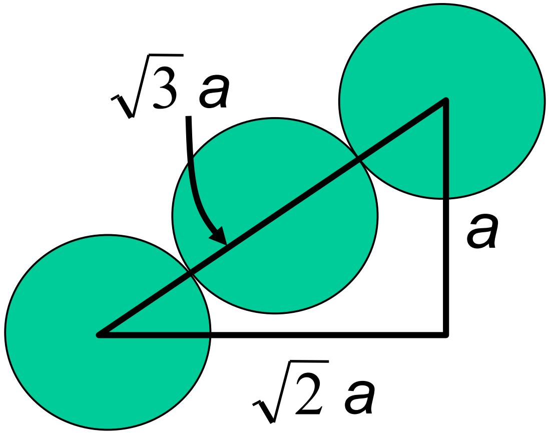
Coordination N = 8



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

Atomic Packing Factor: BCC





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

atoms / unit cell → 2

volume / atom → $\frac{4}{3}\pi(\sqrt{3}a/4)^3$

volume / unit cell → a^3

$$\text{APF} = \frac{2\ \frac{4}{3}\pi\left(\sqrt{3}a/4\right)^3}{a^3} = \text{APF BCC} = 0.68$$

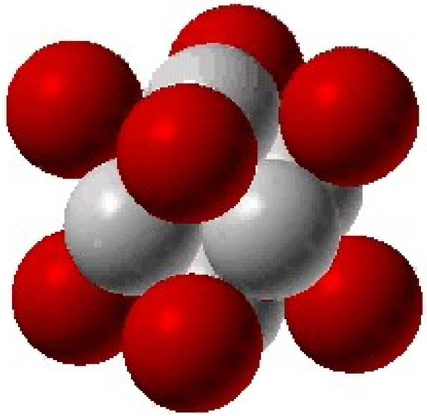
Face Centered Cubic Structure (FCC)

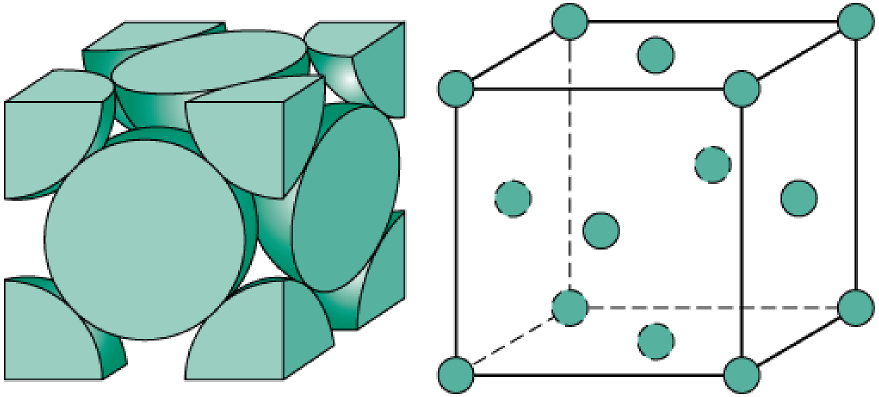
- Atoms touch each other along face diagonals.

Note: All atoms are identical

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

Coordination N = 12



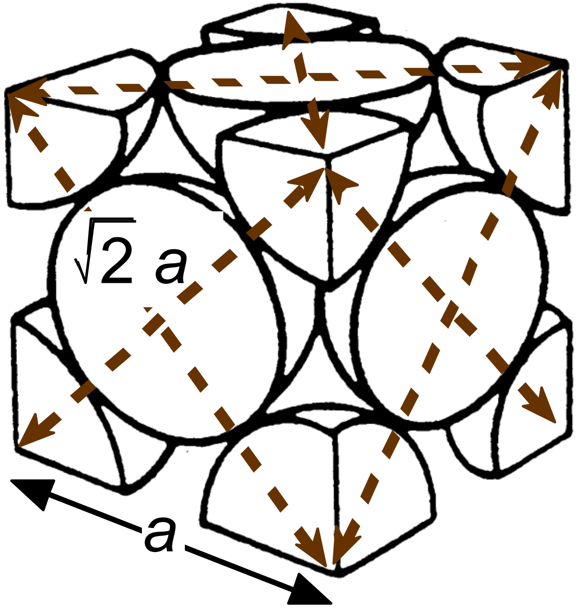


4 atoms/unit cell=6 face x 1/2 + 8 corners x 1/8

Atomic Packing Factor: FCC

maximum achievable APF

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



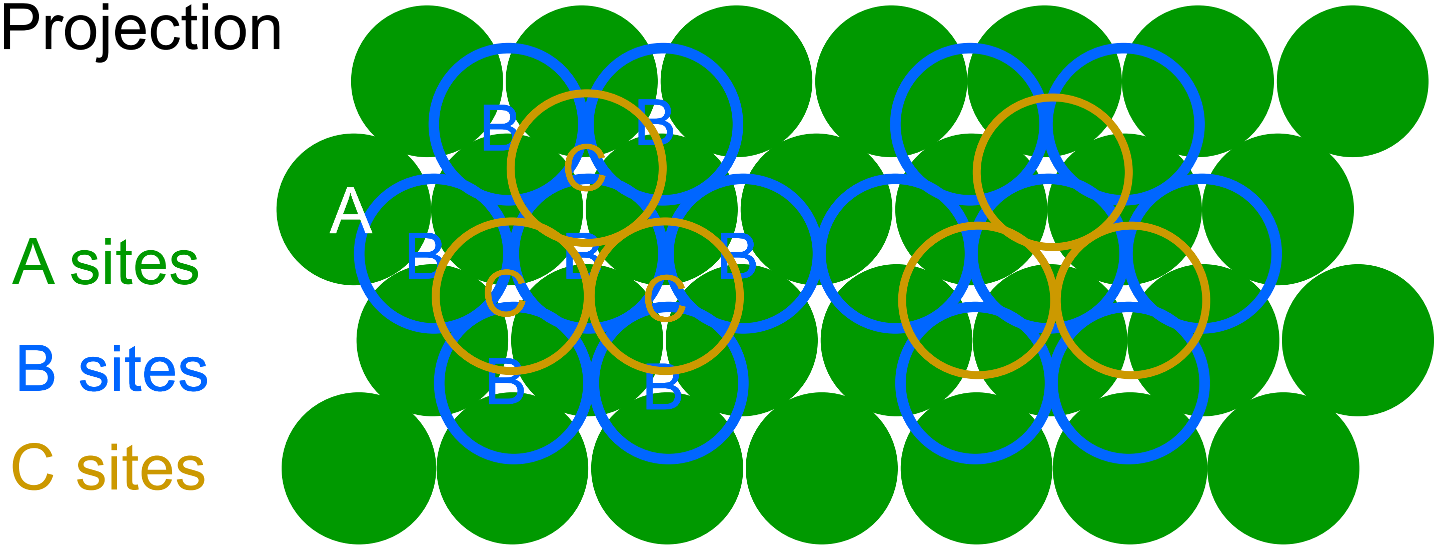
$\frac{\text{atoms}}{\text{unit cell}}$ $\frac{\text{volume}}{\text{atom}}$

$$\text{APF} = \frac{4\ \frac{4}{3}\pi\left(\sqrt{2}a/4\right)^3}{a^3} = \text{APF FCC} = 0.74$$

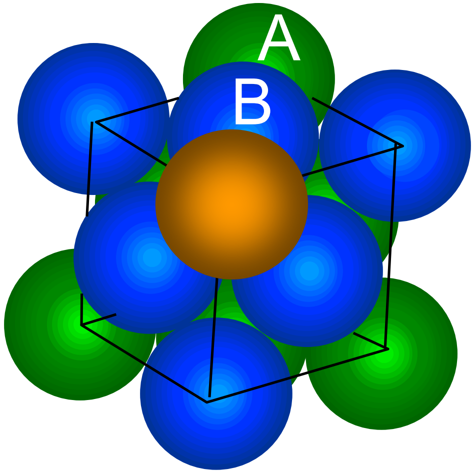
$\frac{\text{volume}}{\text{unit cell}}$

FCC Stacking Sequence

- ABCABC... Stacking Sequence
- 2D Projection

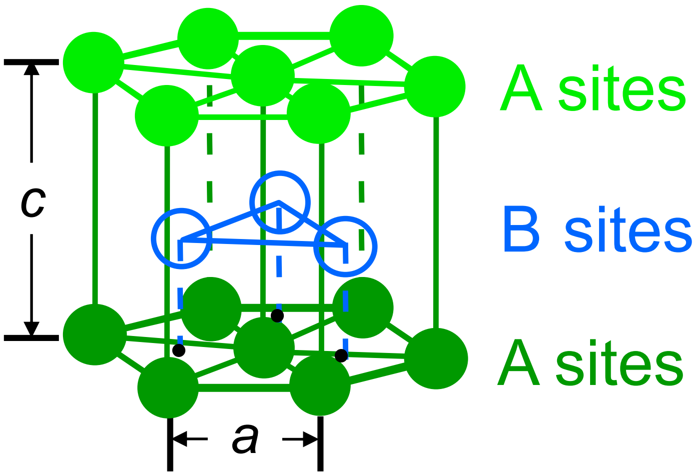


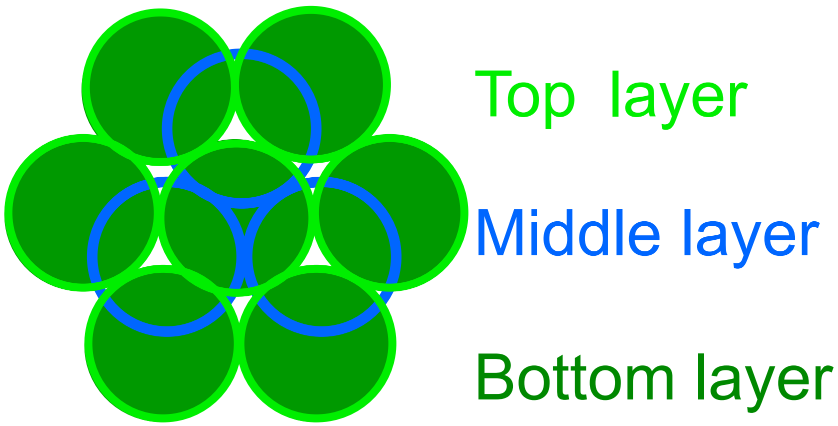
- FCC Unit Cell



Hexagonal Close-Packed Structure (HCP)

- ABAB... Stacking Sequence





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

6 atoms/unit cell

ex: Cd, Mg, Ti, Zn

Polymorphism

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

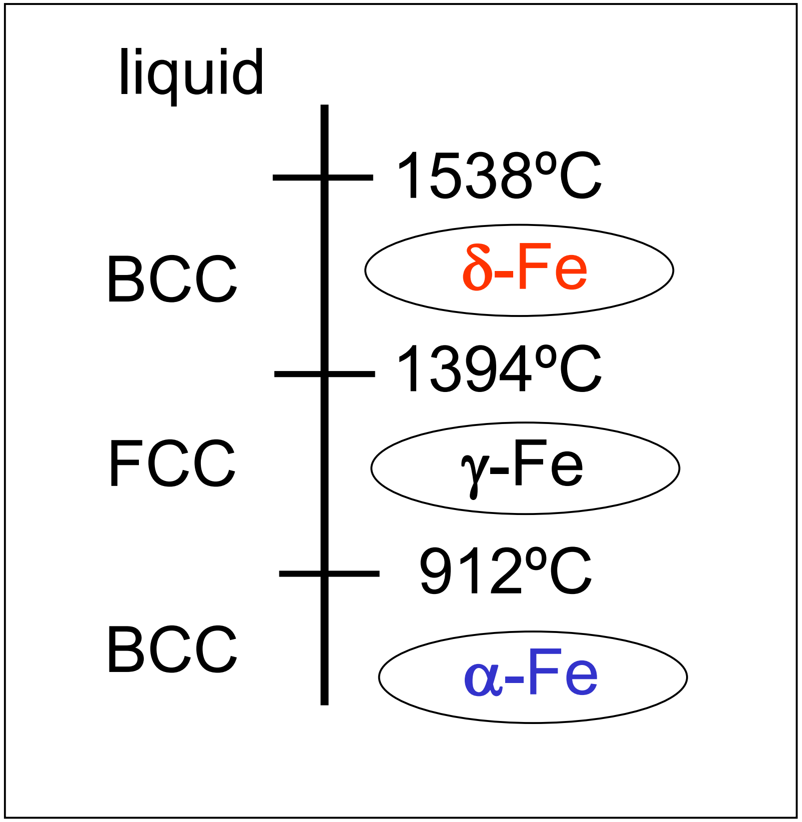
titanium

α, β-Ti

carbon

diamond, graphite

iron system



liquid

1538°C

BCC δ-Fe

1394°C

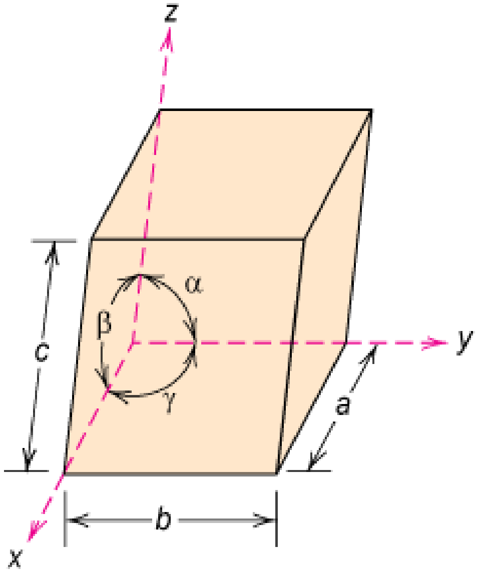
FCC γ-Fe

912°C

BCC α-Fe

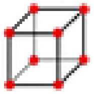
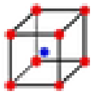
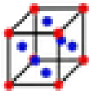
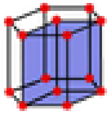
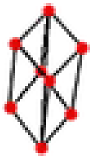
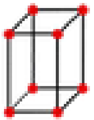
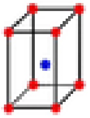
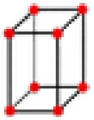
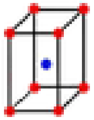
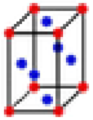
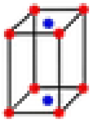
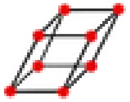
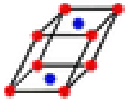
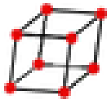
7 crystal systems

14 crystal lattices

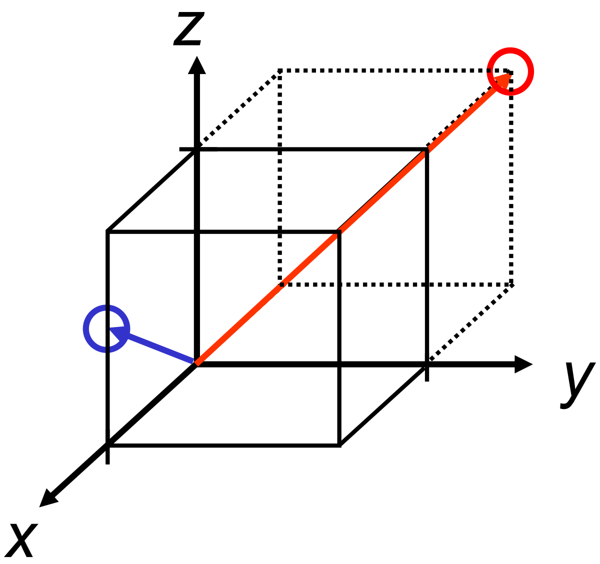


Motif

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

سیستم بلوری	پارامتر های شبکه	ساده	مرکز پر	مرکز وجوه پر	قاعده مرکز دار
مکعبی	$a=b=c$ $\alpha = \beta = \gamma = 90^\circ$				
هگزاگونال	$a_1=a_2=a_3\neq c$ $\alpha_1=\alpha_2=\alpha_3=120,\ \gamma=90^\circ$				
رومبوهدرال	$a=b=c$ $\alpha = \beta = \gamma \neq 90^\circ$				
تتراگونال	$a=b\neq c$ $\alpha = \beta = \gamma = 90^\circ$				
اورتورومبیک	$a\neq b\neq c$ $\alpha = \beta = \gamma = 90^\circ$				
مونوکلینیک	$a\neq b\neq c$ $\alpha = \beta = 90^\circ \neq \gamma$				
تری کلینیک	$a\neq b\neq c$ $\alpha \neq \beta \neq \gamma \neq 90^\circ$				

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

$[uvw]$

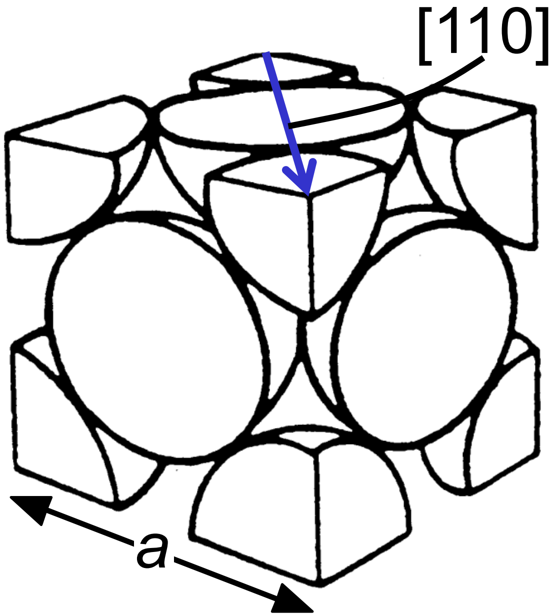
ex: 1, 0, ½ => 2, 0, 1 => [201]

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

families of directions $<uvw>$

Linear Density

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



Adapted from Fig. 3.1(a), *Callister & Rethwisch 8e.*

ex: linear density of Al in [110] direction

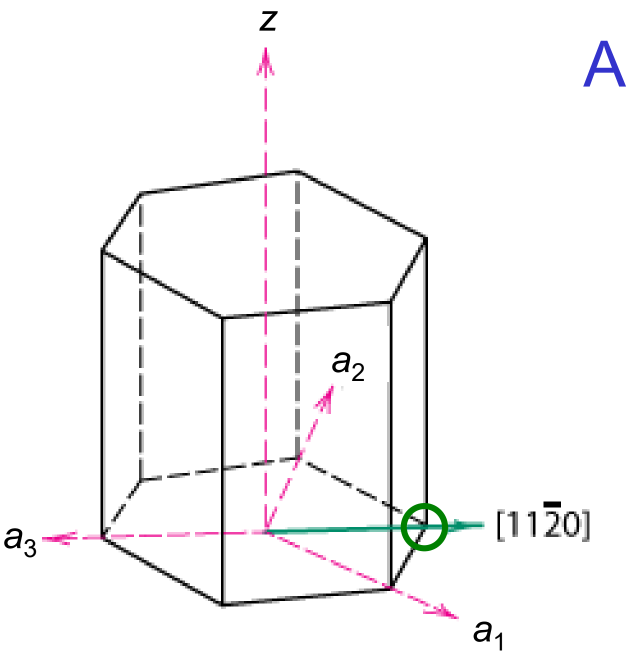
a = 0.405 nm

atoms

length

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

HCP Crystallographic Directions



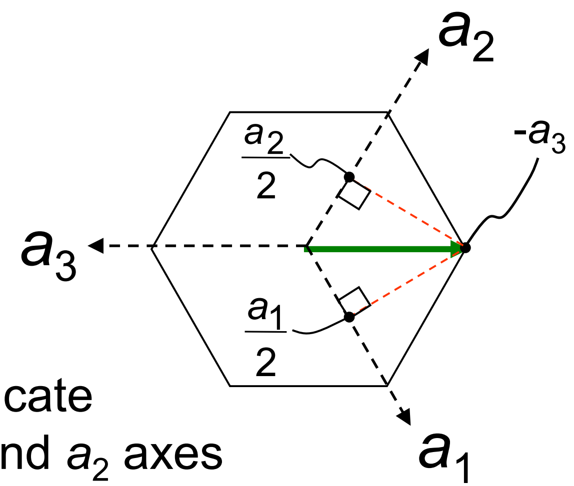
Adapted from Fig. 3.8(a), *Callister & Rethwisch 8e.*

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

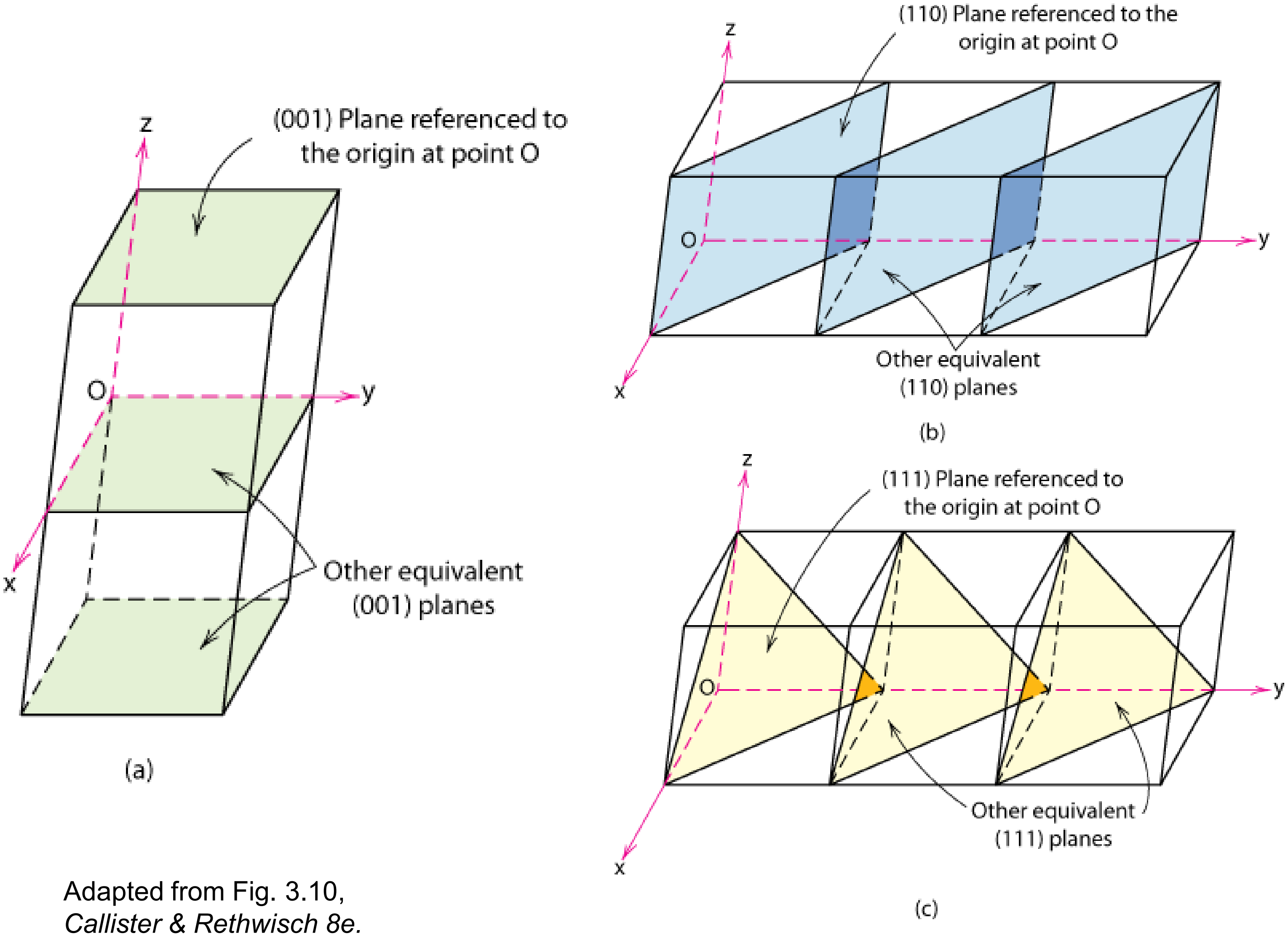
$[uvtw]$

ex: ½, ½, -1, 0 => $[11\bar{2}0]$



dashed red lines indicate projections onto a_1 and a_2 axes

Crystallographic Planes



(a) (b) (c)

Adapted from Fig. 3.10, *Callister & Rethwisch 8e.*

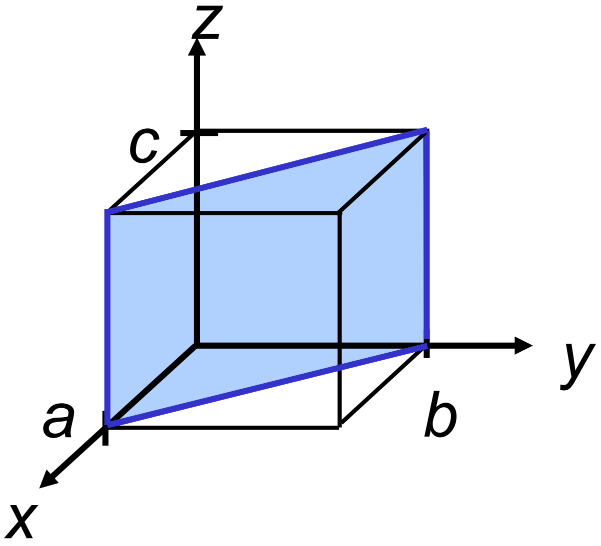
Crystallographic Planes

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

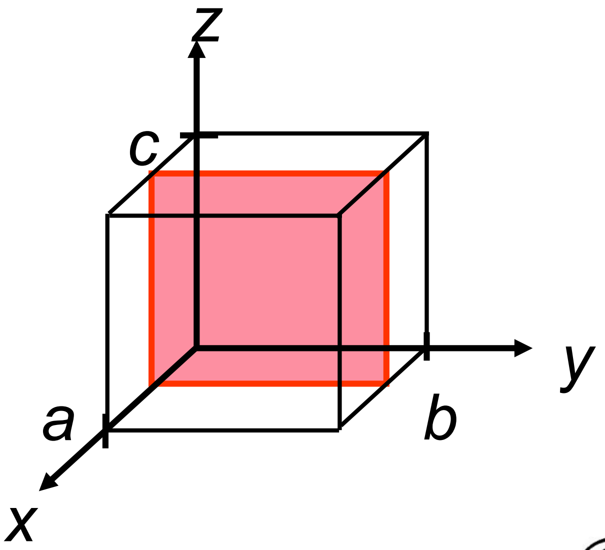
- Algorithm
  1. Read off intercepts of plane with axes in terms of *a*, *b*, *c*
  2. Take reciprocals of intercepts
  3. Reduce to smallest integer values
  4. Enclose in parentheses, no commas i.e., (*hkl*)

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)		

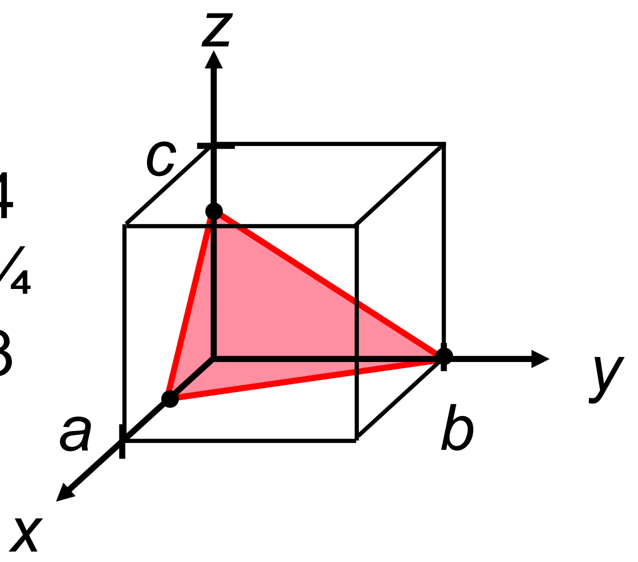


example	*a*	*b*	*c*
1. Intercepts	1/2	∞	∞
2. Reciprocals	1/½	1/∞	1/∞
	2	0	0
3. Reduction	2	0	0
4. Miller Indices	(100)		



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*}

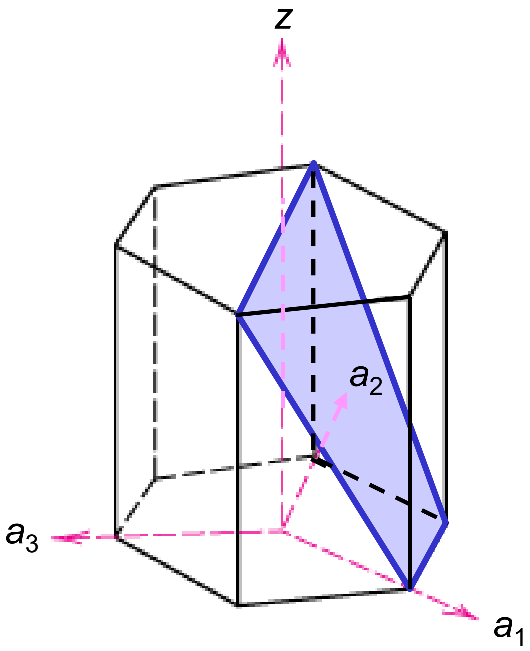
Ex: $\{100\} = (100), (010), (001), (\bar{1}00), (0\bar{1}0), (00\bar{1})$

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

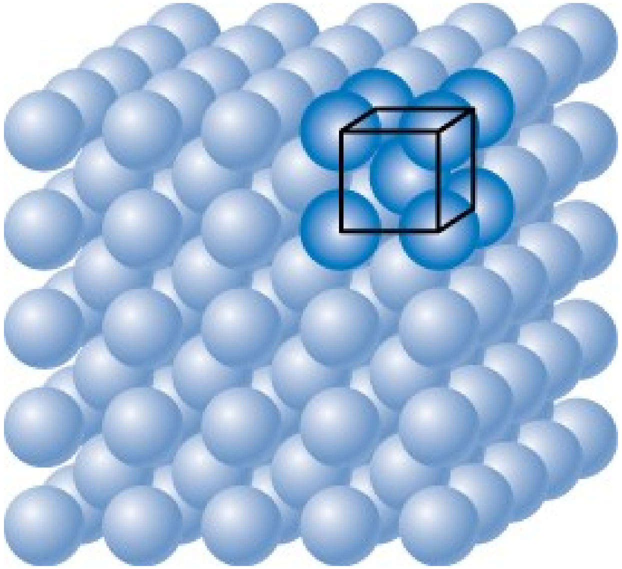
4. Miller-Bravais Indices $(10\bar{1}1)$



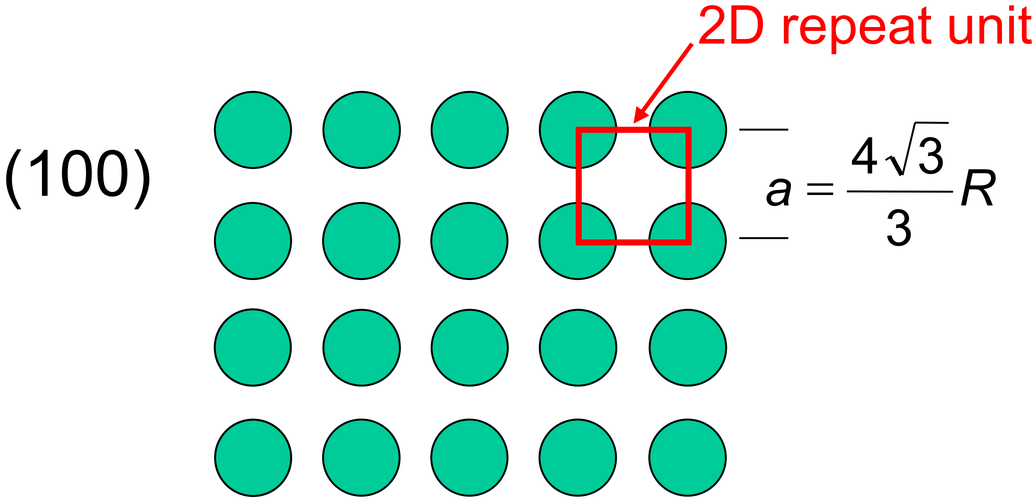
Adapted from Fig. 3.8(b), *Callister & Rethwisch 8e.*

Planar Density of (100) Iron

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



Adapted from Fig. 3.2(c), *Callister & Rethwisch 8e.*



$$a = \frac{4\sqrt{3}}{3}R$$

Radius of iron $R = 0.1241$ nm

$$\frac{\text{atoms}}{\text{2D repeat unit}}$$

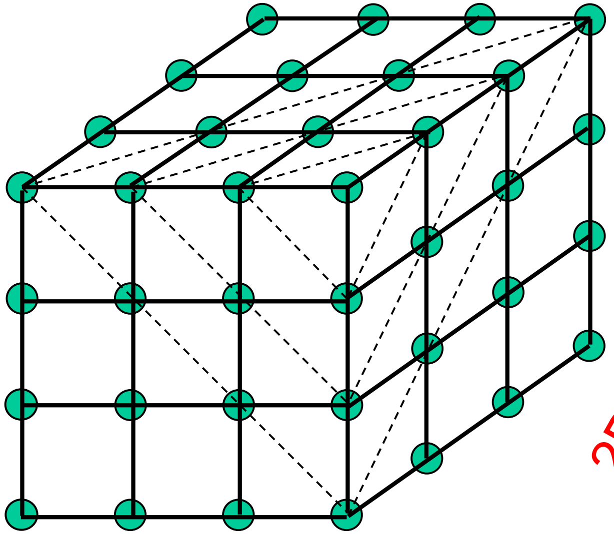
$$\text{Planar Density} = \frac{1}{a^2} = \frac{1}{\left(\frac{4\sqrt{3}}{3}R\right)^2} = 12.1\,\frac{\text{atoms}}{\text{nm}^2} = \boxed{1.2 \times 10^{19}\,\frac{\text{atoms}}{\text{m}^2}}$$

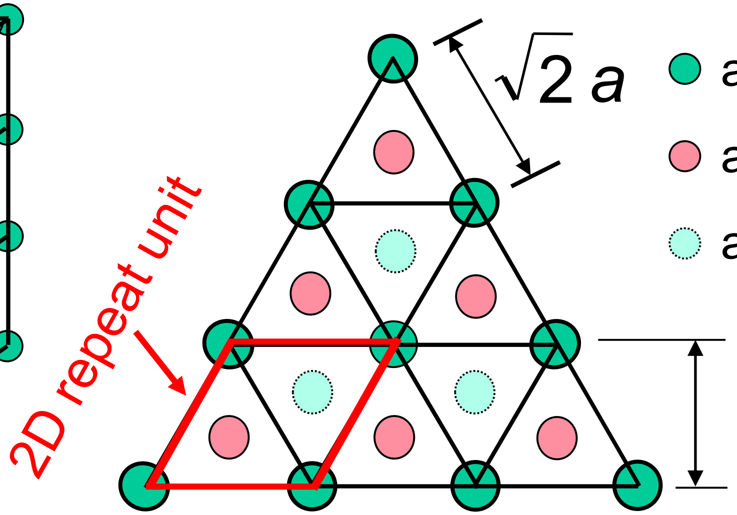
$$\frac{\text{area}}{\text{2D repeat unit}}$$

Planar Density of (111) Iron

Solution (cont): (111) plane

1 atom in plane/ unit surface cell





● atoms in plane

● atoms above plane

○ atoms below plane

$$h = \sqrt{\frac{3}{2}}\,a$$

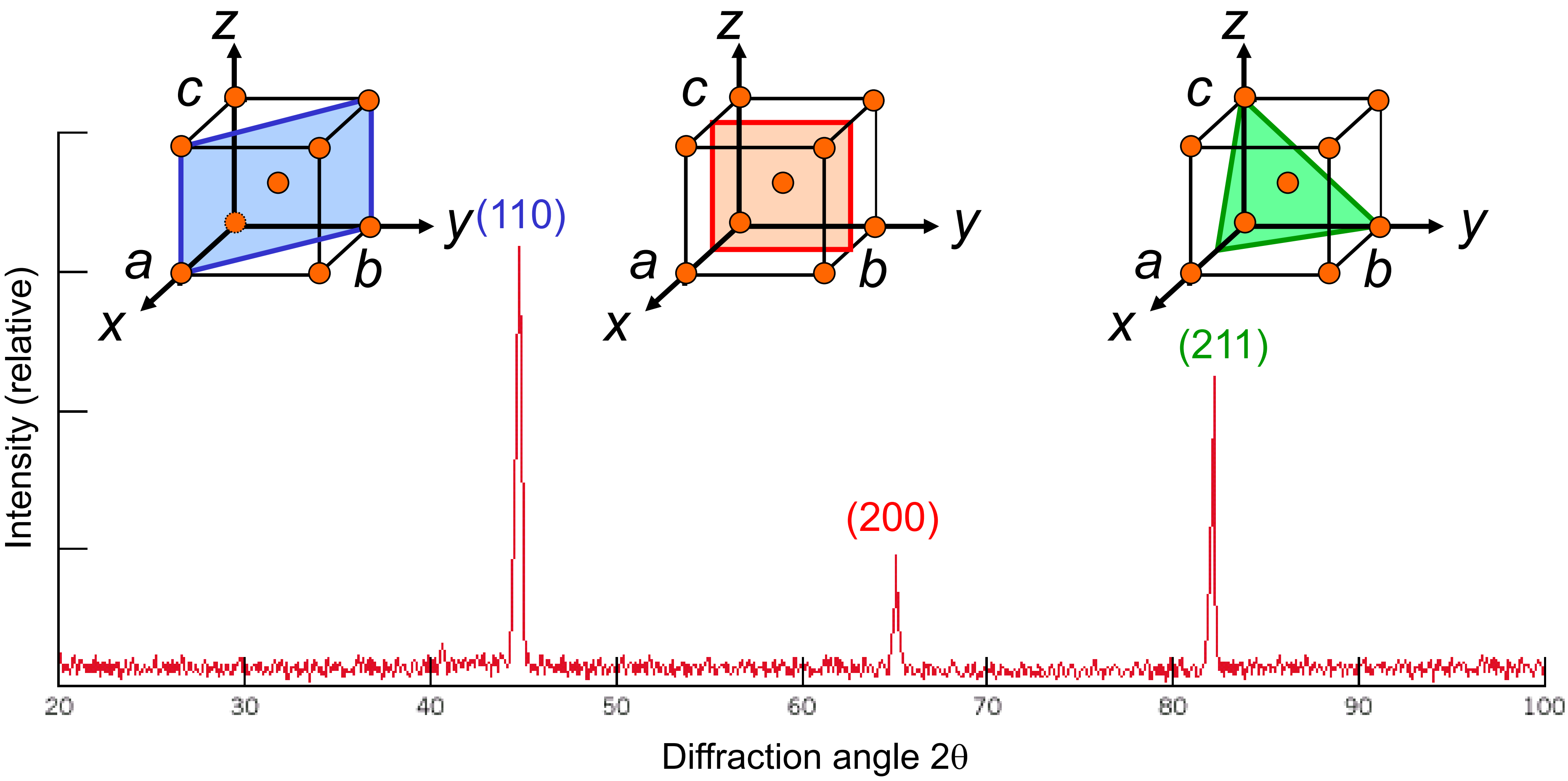
$$\text{area} = \sqrt{2}\,ah = \sqrt{3}\,a^2 = \sqrt{3}\left(\frac{4\sqrt{3}}{3}R\right)^2 = \frac{16\sqrt{3}}{3}R^2$$

$$\text{Planar Density} = \frac{1}{\frac{16\sqrt{3}}{3}R^2} = 7.0\,\frac{\text{atoms}}{\text{nm}^2} = \boxed{0.70 \text{ x } 10^{19}\,\frac{\text{atoms}}{\text{m}^2}}$$

$\dfrac{\text{atoms}}{\text{2D repeat unit}}$ → 1

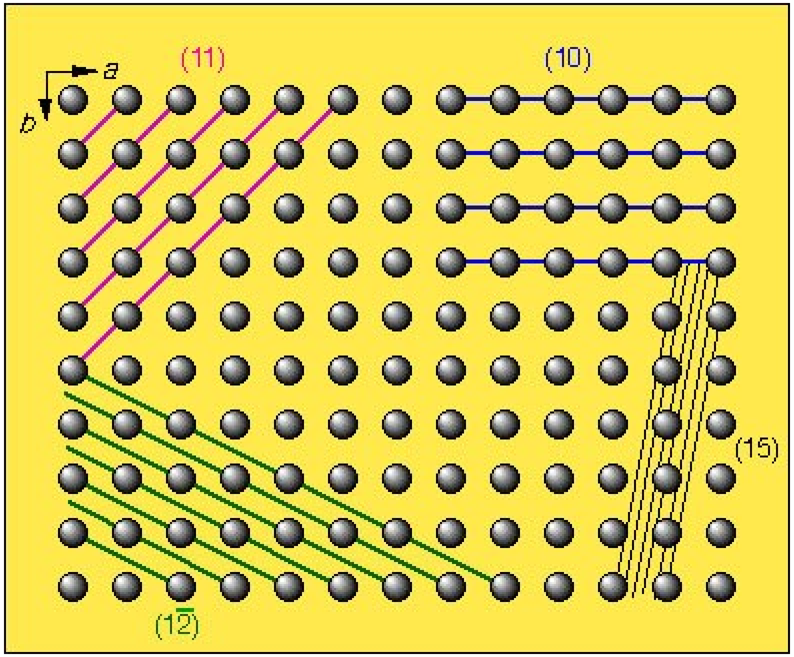
$\dfrac{\text{area}}{\text{2D repeat unit}}$ → $\dfrac{16\sqrt{3}}{3}R^2$

X-Ray Diffraction Pattern



Diffraction pattern for polycrystalline α-iron (BCC)

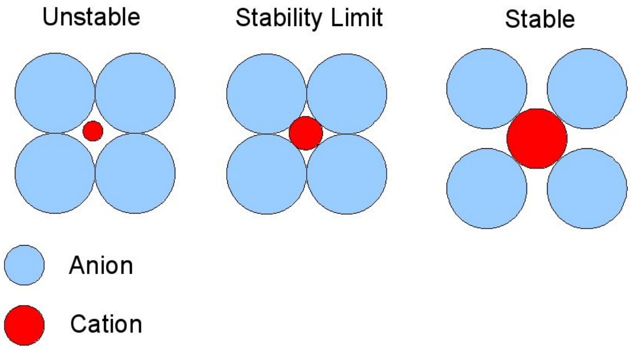
Adapted from Fig. 3.22, *Callister 8e.*

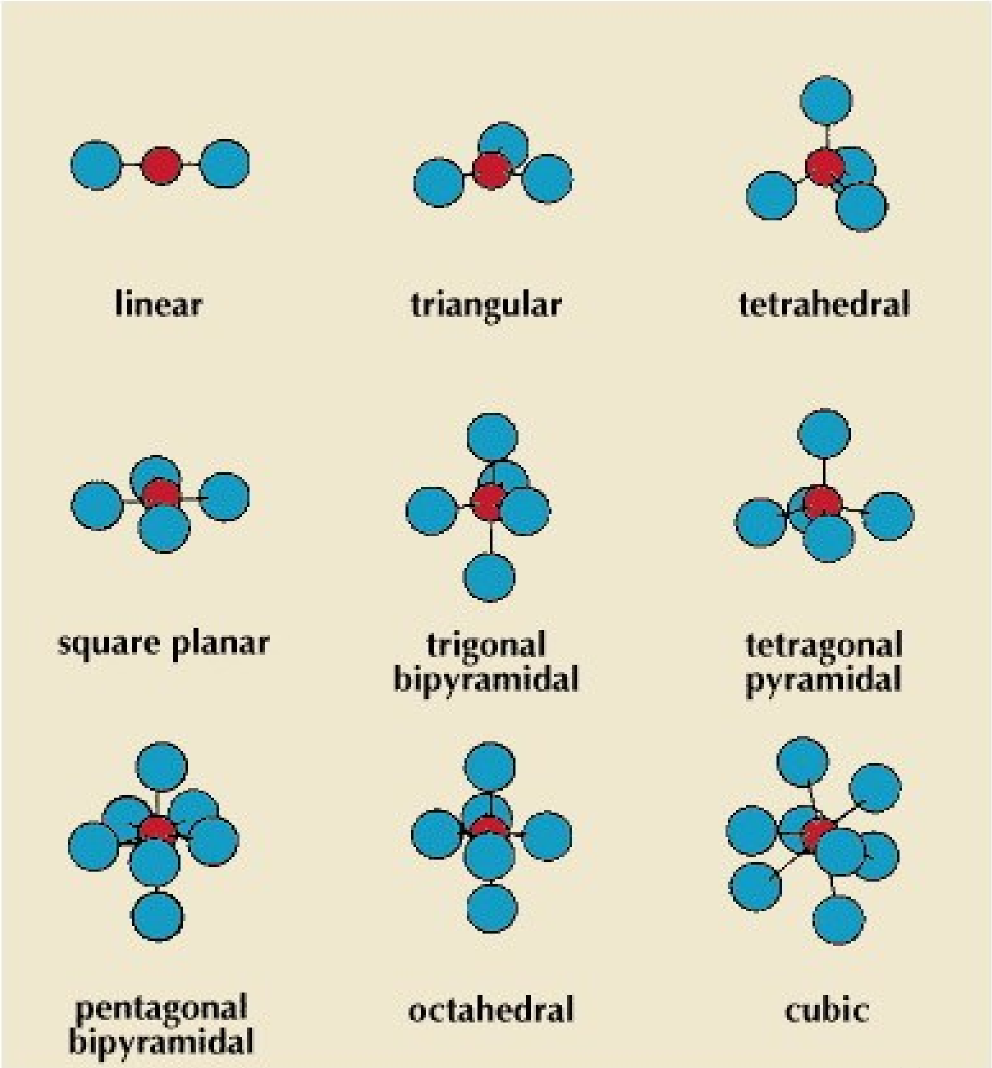

a
b
(11)
(10)
(15)
$(1\bar{2})$

Structure	a_0 vs. r	Atoms per cell	Coordination Number	Packing factor	Examples
SC	$a_0 = 2r$	1	6	0.52	Polonium (Po),α-Mn
BCC	$a_0 = \frac{4}{\sqrt{3}} r$	2	8	0.68	Fe,Ti,W,Mo, Nb,Ta,K,Na, V,Zr,Cr
FCC	$a_0 = \frac{4}{\sqrt{2}} r$	4	12	0.74	Fe,Cu,Au,Pt ,Ag,Pb,Ni
HCP	$a_0 = 2r$ $c_0 \approx 1.633 a_0$	2	12	0.74	Ti,Mg,Zn,Be ,Co,Zr,Cd

Predicting Crystal Structures

CN	r^+/r^-
8	≥0.732
6	≥ 0.414
4	≥ 0.225
3	≥ 0.155





Interstices in typical crystals of metals

Definition:

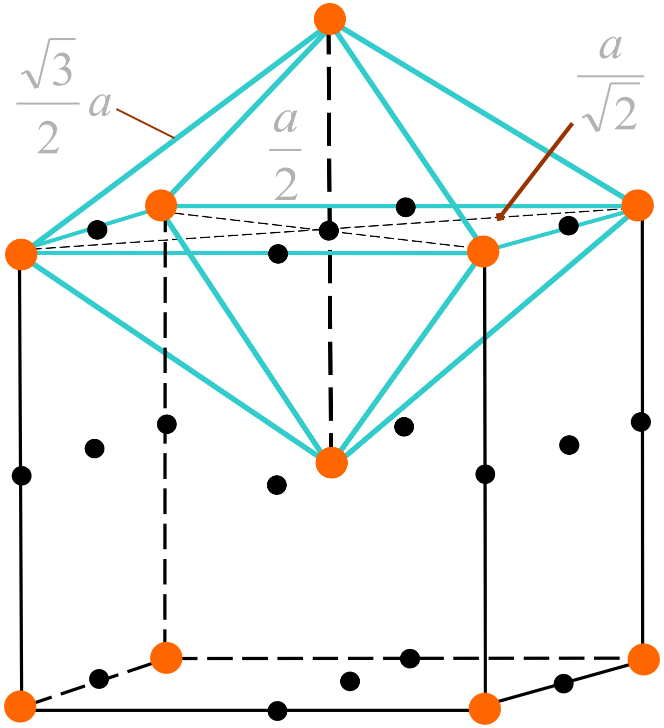
In any of the crystal structures, there are small holes between the usual atoms into which smaller atoms may be placed. These locations are called interstitial sites.

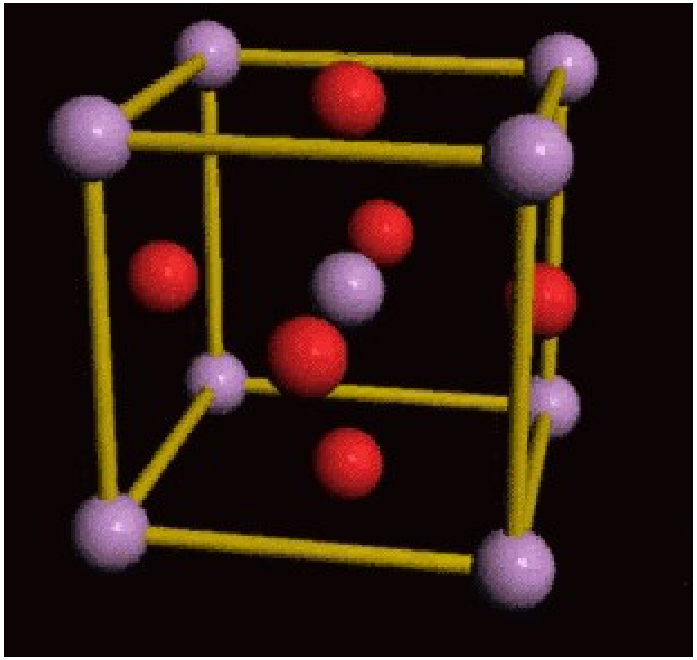
I. Two types of Interstitials in typical crystals

$\begin{cases} \text{Octahedral interstitial} \\ \text{Tetrahedral interstitial} \end{cases}$

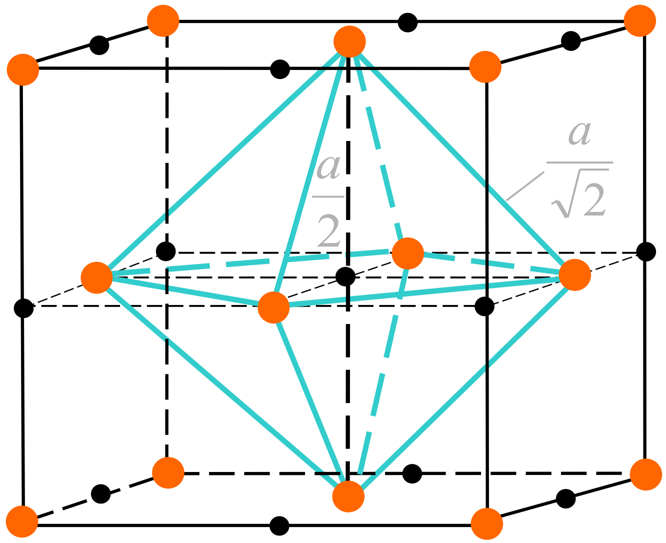
1. Octahedral interstitial

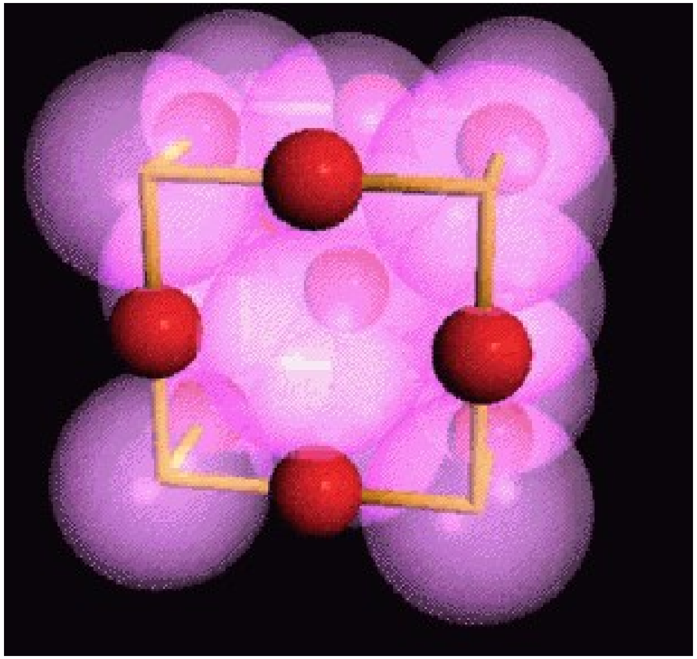
BCC



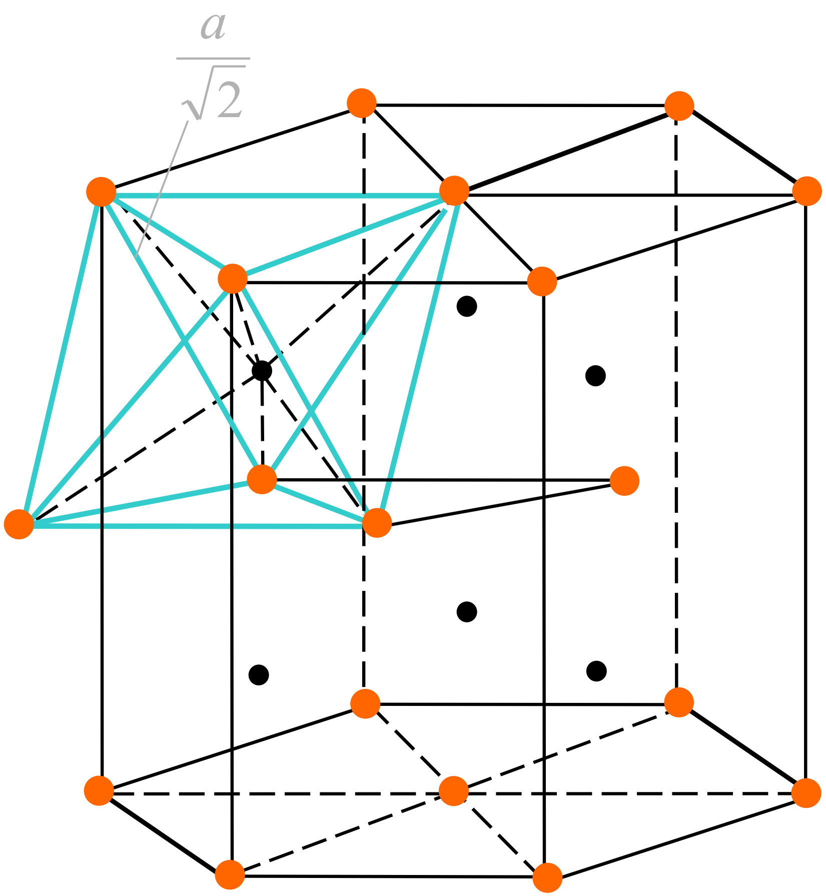


FCC



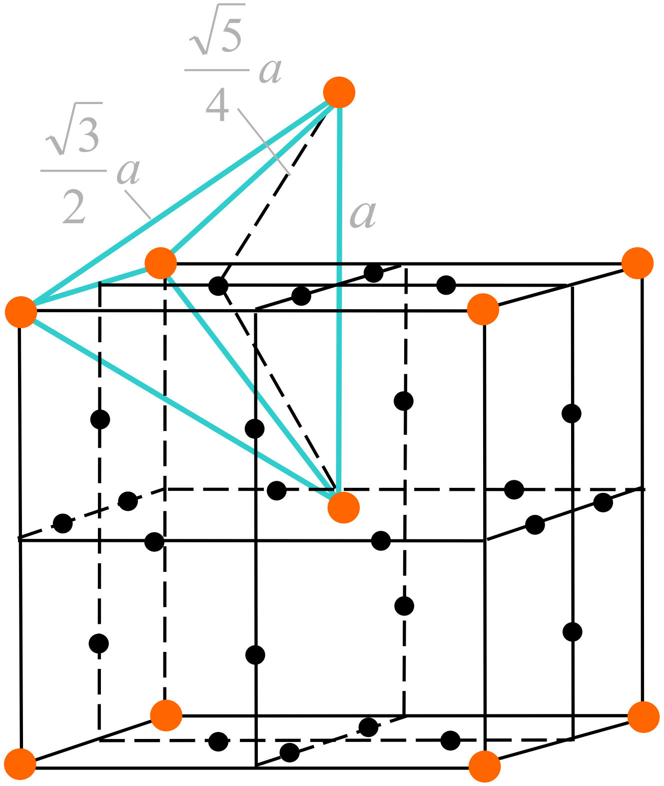


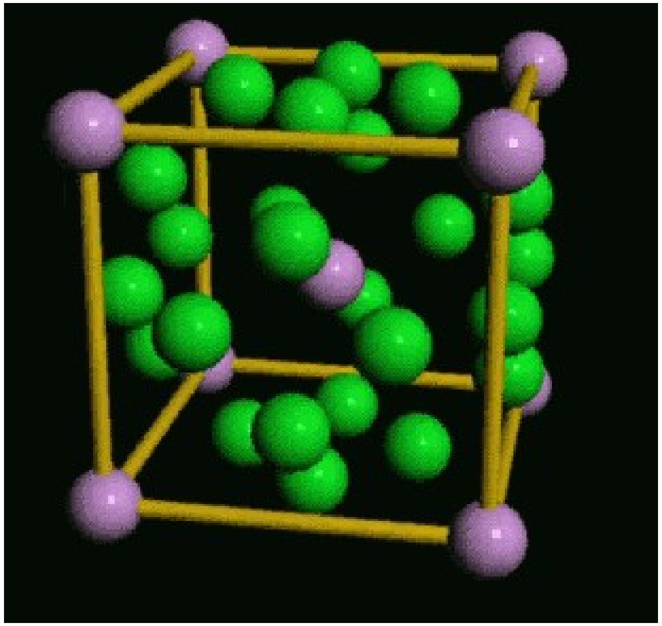
HCP



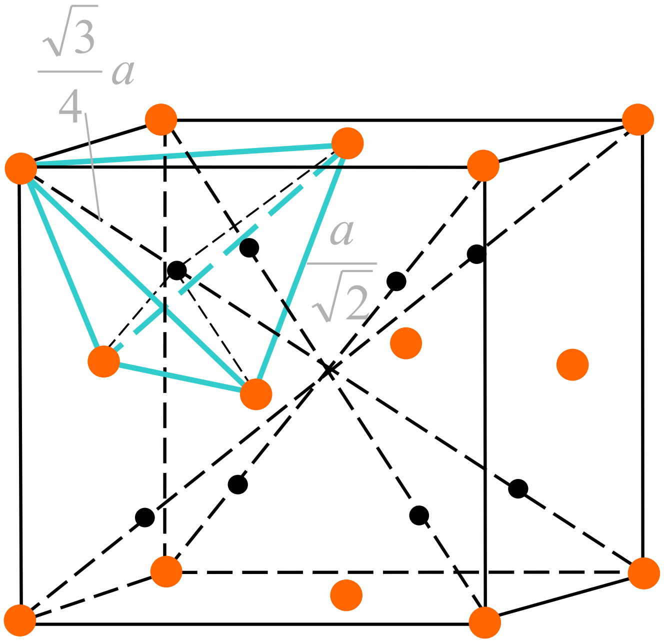
2. Tetrahedral interstitial

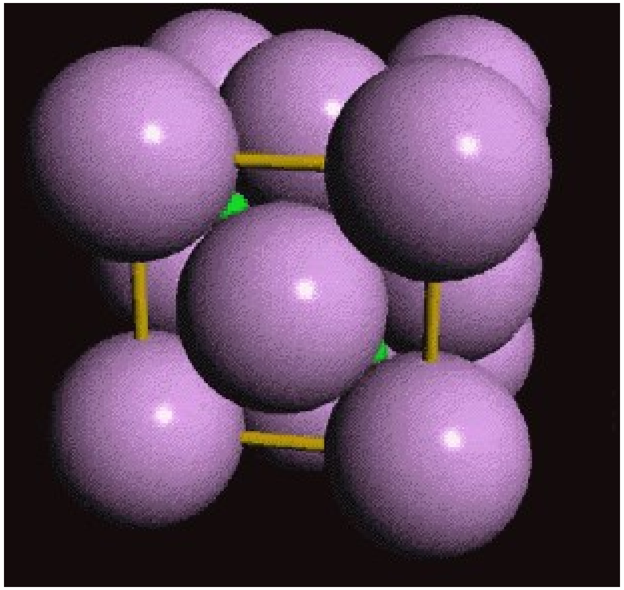
BCC



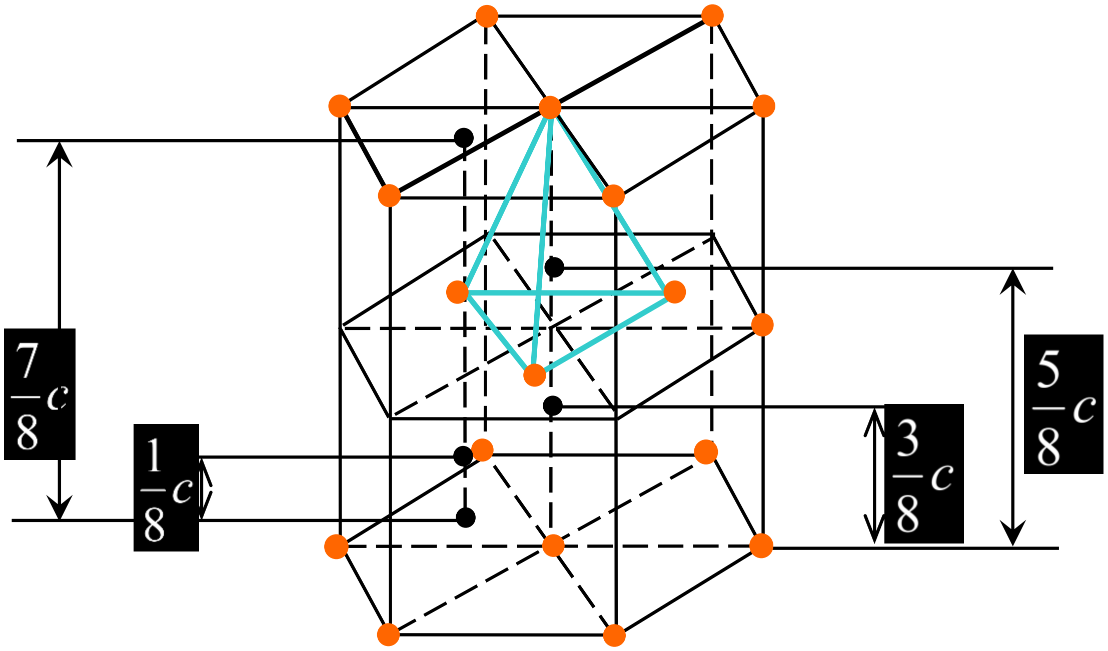


FCC





HCP



Summary

	n	CN	ξ	interstices				d_i/d_a	
				oct.		tete.		oct.	tete.
BCC	2	8	0.68	6	6/2=3	12	12/2=6	0.15	0.29
FCC	4	12	0.74	4	4/4=1	8	8/4=2	0.41	0.22
HCP	6	12	0.74	6	6/6=1	12	12/6=2	0.41	0.22

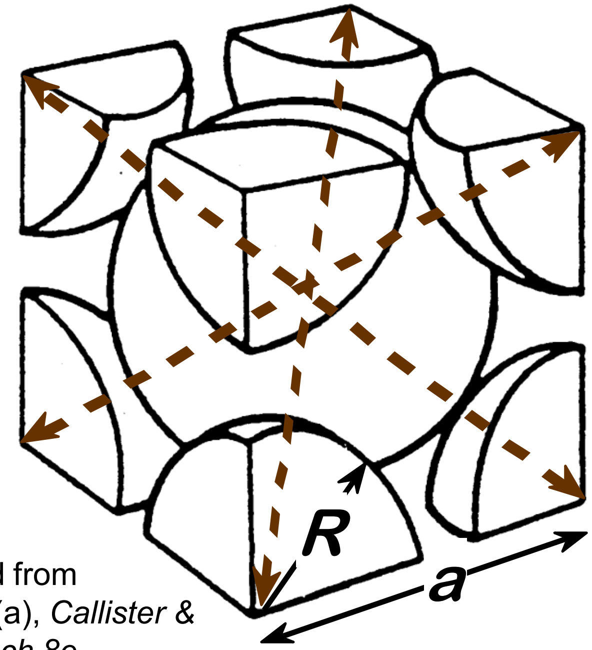
Theoretical Density, ρ

$$\text{Density} = \rho = \frac{\text{Mass of Atoms in Unit Cell}}{\text{Total Volume of Unit Cell}}$$

$$\rho = \frac{n\,A}{V_C N_A}$$

where n = number of atoms/unit cell
A = atomic weight
V_C = Volume of unit cell = a^3 for cubic
N_A = Avogadro's number
= 6.022×10^{23} atoms/mol

Theoretical Density, ρ



Adapted from Fig. 3.2(a), *Callister & Rethwisch 8e.*

- Ex: Cr (BCC)

  A = 52.00 g/mol

  R = 0.125 nm

  n = 2 atoms/unit cell

  $a = 4R/\sqrt{3} = 0.2887$ nm

$$\rho = \frac{\overset{\frac{\text{atoms}}{\text{unit cell}}}{2}\ \overset{\frac{\text{g}}{\text{mol}}}{52.00}}{\underset{\frac{\text{volume}}{\text{unit cell}}}{a^3}\ \underset{\frac{\text{atoms}}{\text{mol}}}{6.022 \times 10^{23}}}$$

$\rho_{\text{theoretical}}$ = 7.18 g/cm^3

ρ_{actual} = 7.19 g/cm^3

Determine the density of BCC iron, which has a lattice parameter of 0.2866nm.

Solution:

For a BCC cell, Atoms/cell = 2

$$a_0 = 0.2866\text{nm} = 2.866 \times 10^{-8}\text{cm}$$

$$\text{Atomic mass} = 55.847\text{g/mol}$$

$$\text{Volume of unit cell} = a_0^3 = 23.54 \times 10^{-24}\text{cm}^3/\text{cell}$$

$$\text{Density} \quad \rho = \frac{(\text{number of atoms / cell})(\text{atomic mass of iron})}{(\text{volume of unit cell})(\text{Avogadro's number})}$$

$$= \frac{(2)(55.847)}{(23.54 \times 10^{-24})(6.02 \times 10^{23})} = 7.882\text{g / cm}^3$$

Densities of Material Classes

In general

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

Why?

Metals have...

- close-packing (metallic bonding)
- often large atomic masses

Ceramics have...

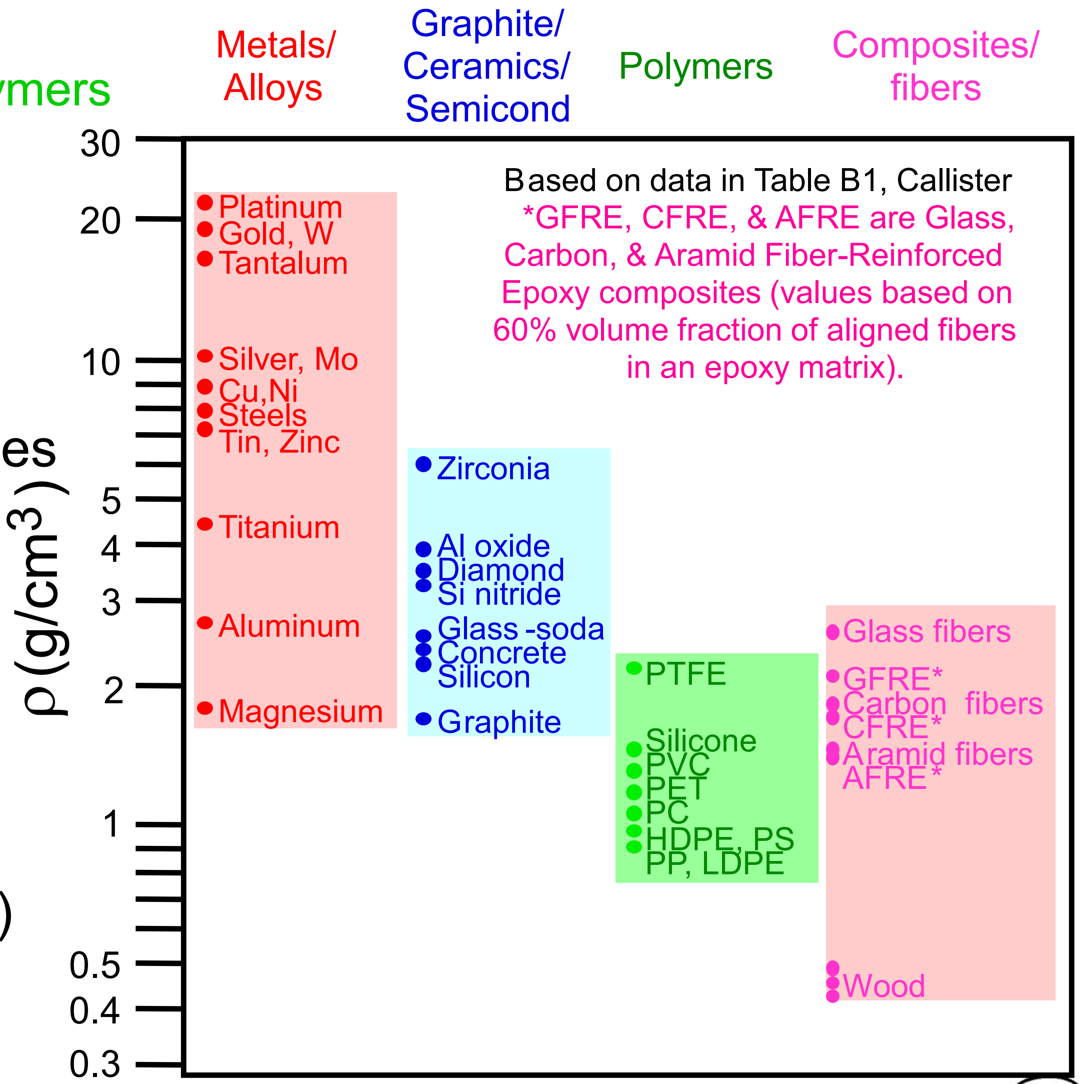
- less dense packing
- often lighter elements

Polymers have...

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

Composites have...

- intermediate values

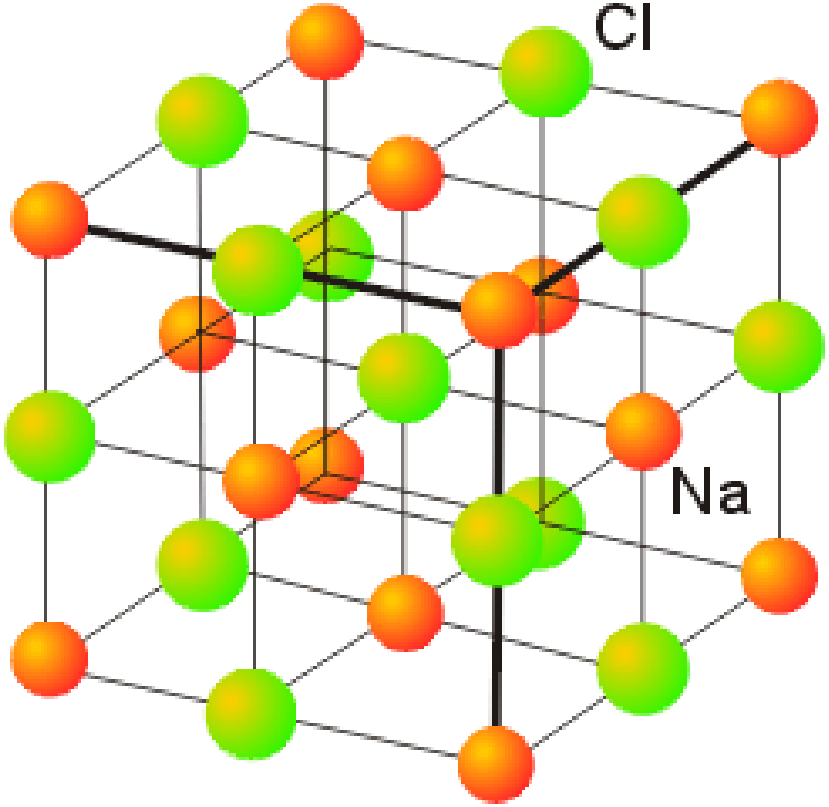


Based on data in Table B1, Callister

*GFRE, CFRE, & AFRE are Glass, Carbon, & Aramid Fiber-Reinforced Epoxy composites (values based on 60% volume fraction of aligned fibers in an epoxy matrix).

Data from Table B.1, *Callister & Rethwisch, 8e.*

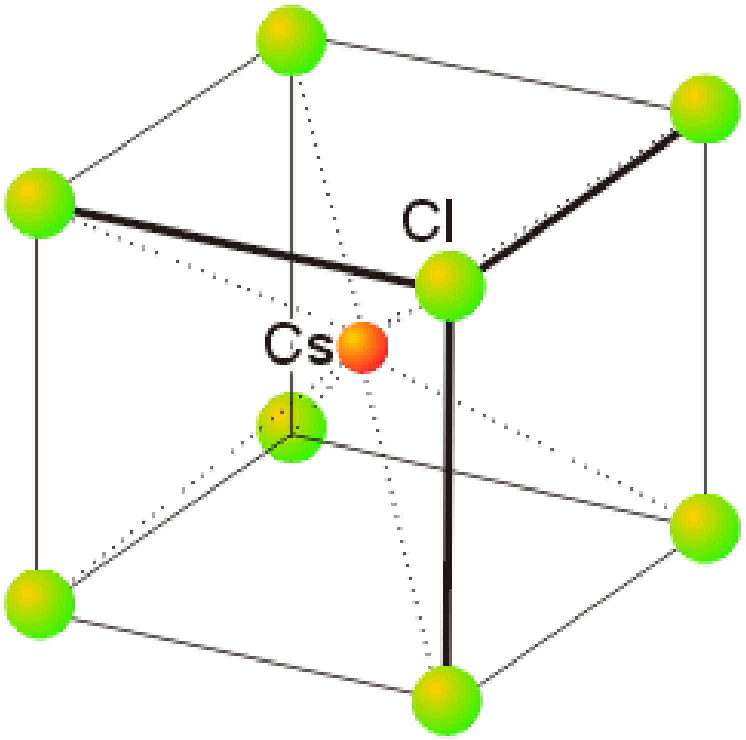
Common Crystal Types



1. The Rock Salt (NaCl) structure-

   The coordination number is 6 for both ions.

Common Crystal Types



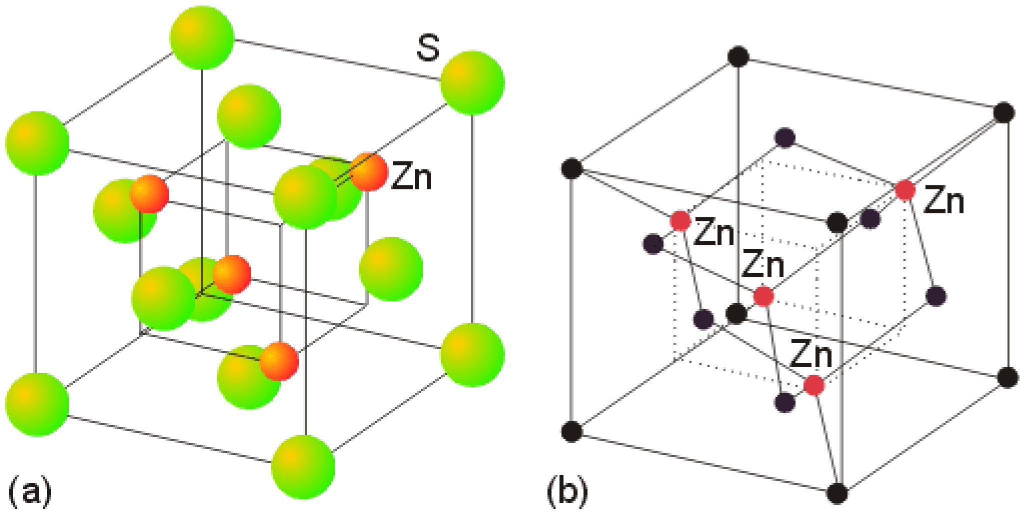
2. The CsCl structure-

Chloride ions occupy the corners of a cube, with a cesium ion in the center (called a *cubic hole*) or vice versa. Both ions have a coordination number of 8, with the two ions fairly similar in size.

Common Crystal Types

3. The Zinc-blende or ZnS structure

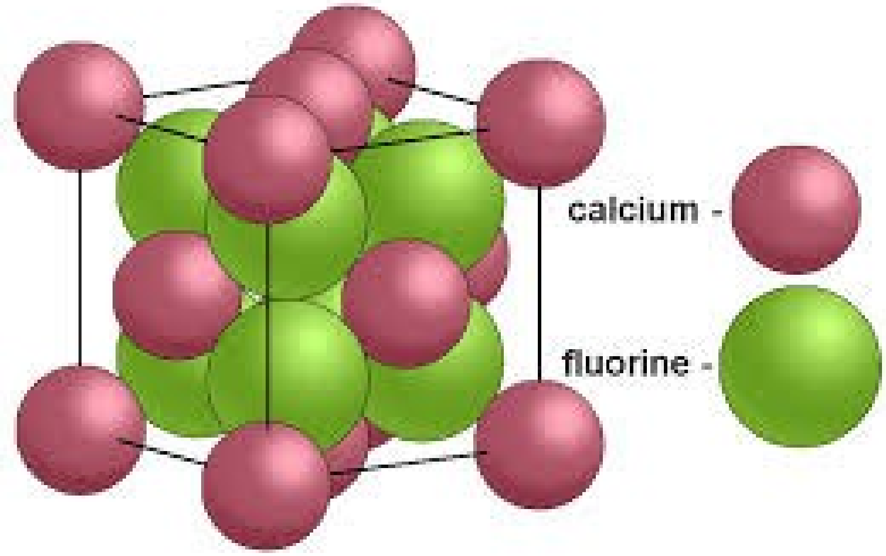
Anions (S^{2-}) ions are in a face-centered cubic arrangement, with cations (Zn^{2+}) in half of the tetrahedral holes.

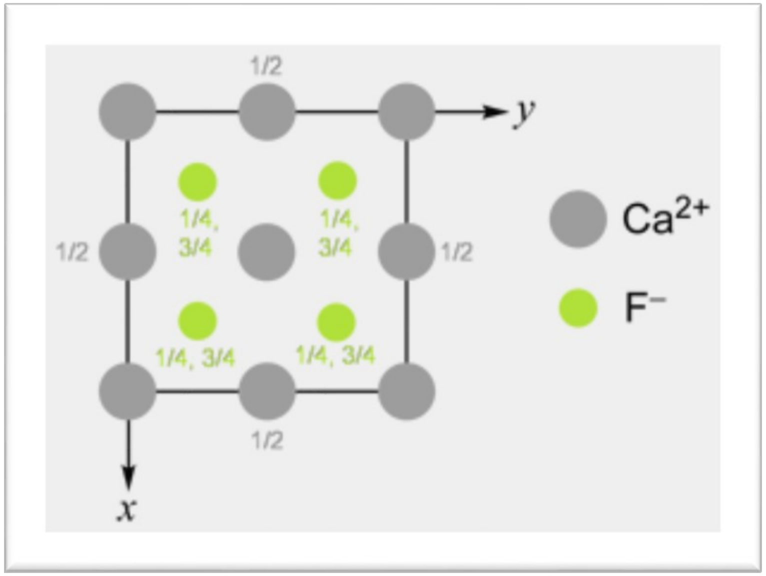


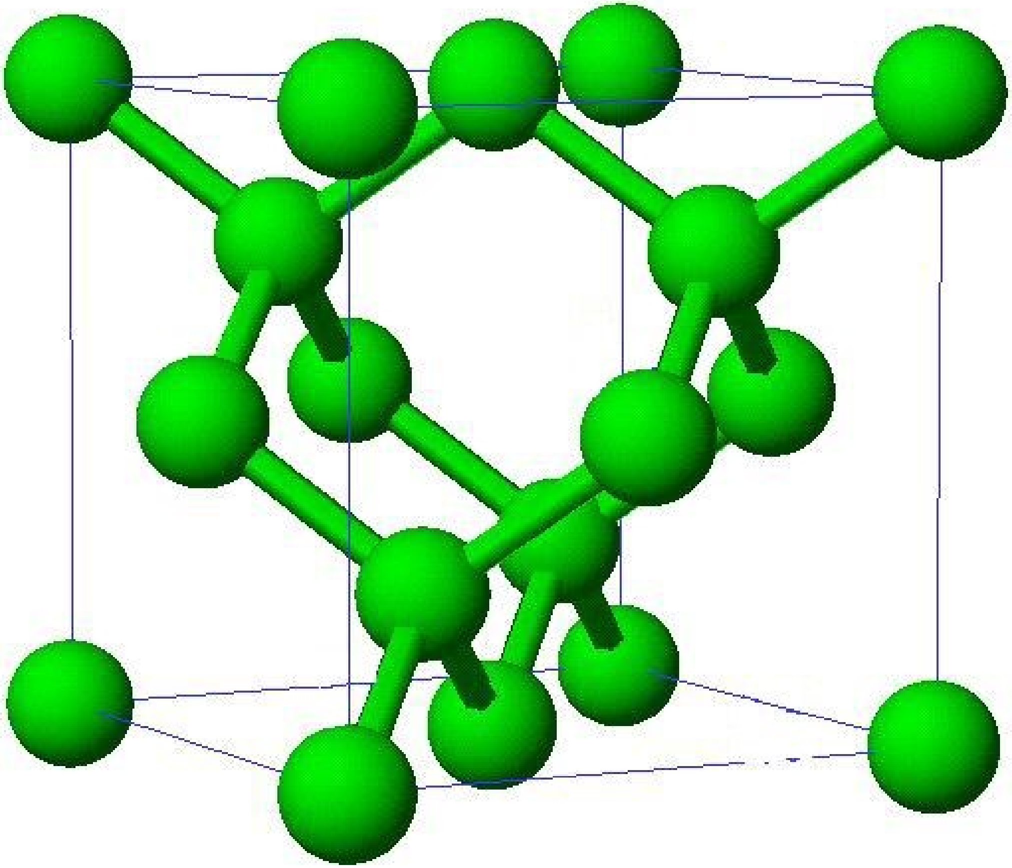
Common Crystal Types

4. The Fluorite (CaF_2) : A face-centered cubic arrangement of Ca^{2+} ions with F^- ions in <u>all</u> of the tetrahedral holes.

5. The antifluorite structure reverses the positions of the cations and anions. An example is K_2O.







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Imperfections in Solids

- The properties of some materials are profoundly influenced by the presence of imperfections.
- It is important to have knowledge about the types of imperfections that exist and the roles they play in affecting the behavior of materials.

Types of Imperfections

- Vacancy atoms
- Interstitial atoms
- Substitutional atoms

Point defects

1-2 atoms

- Dislocations

Line defects

1-dimensional

- Grain Boundaries

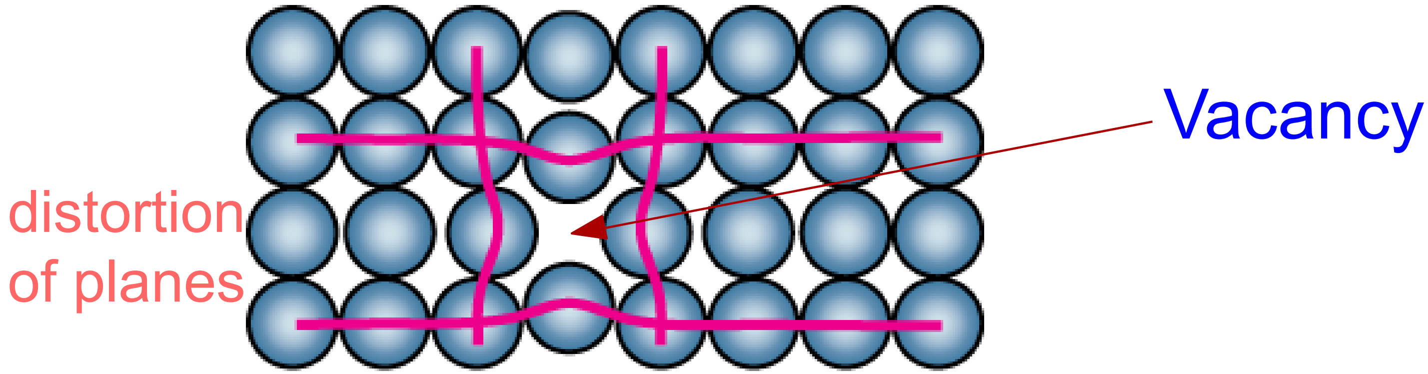
Area defects

2-dimensional

Point Defects in Metals

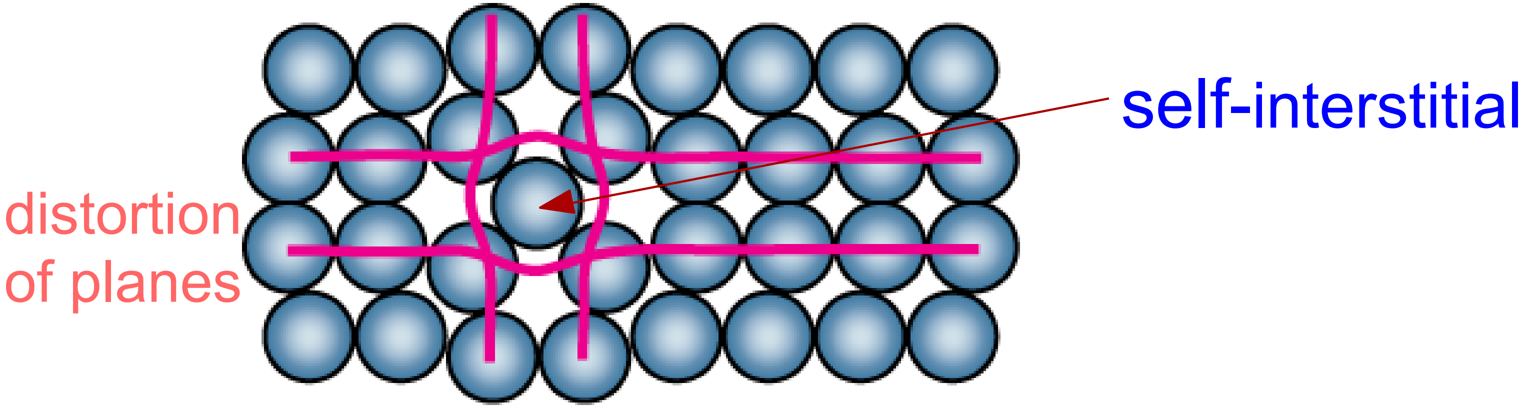
- Vacancies:

  -vacant atomic sites in a structure.

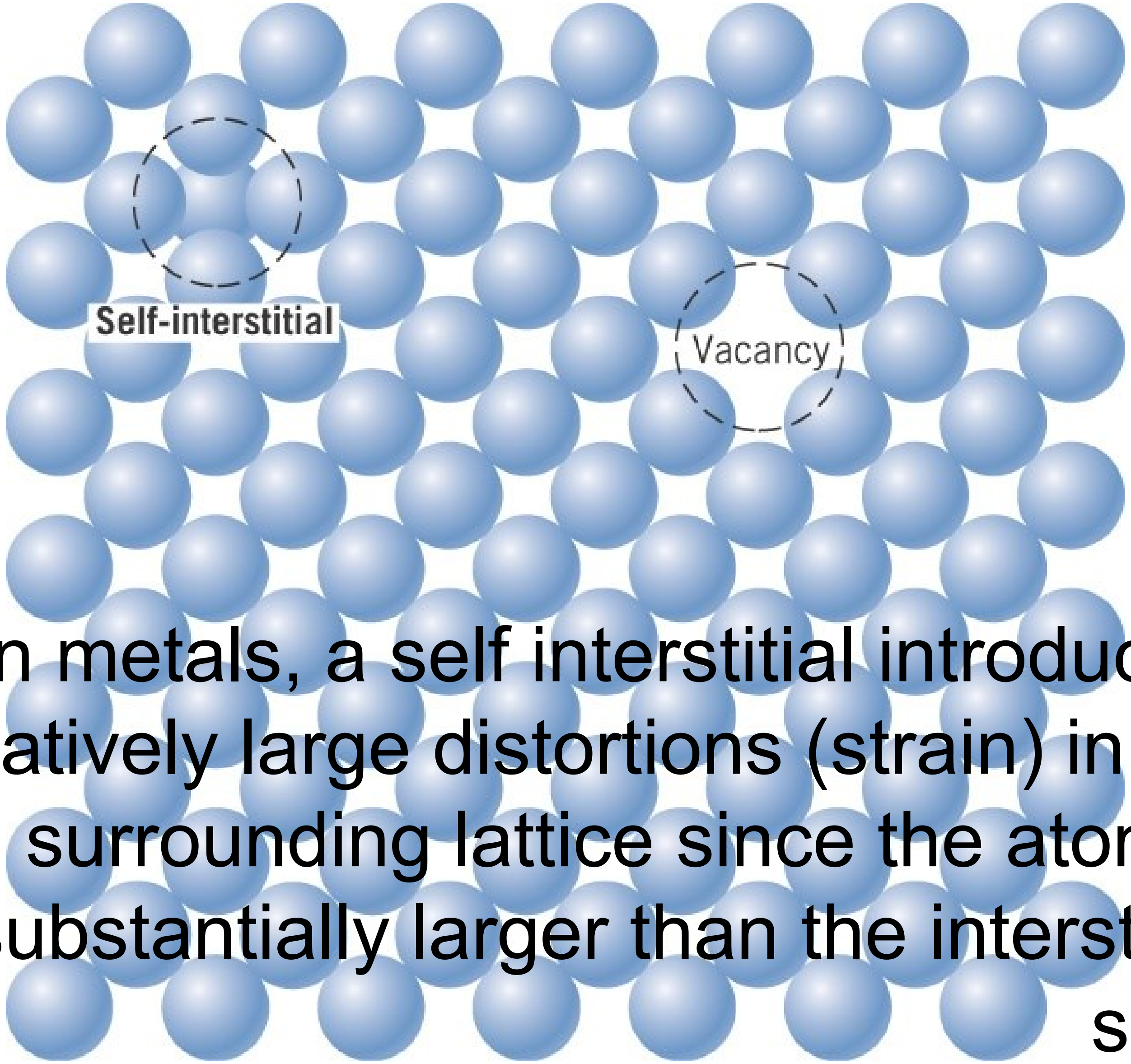


- Self-Interstitials:

  -"extra" atoms positioned between atomic sites.



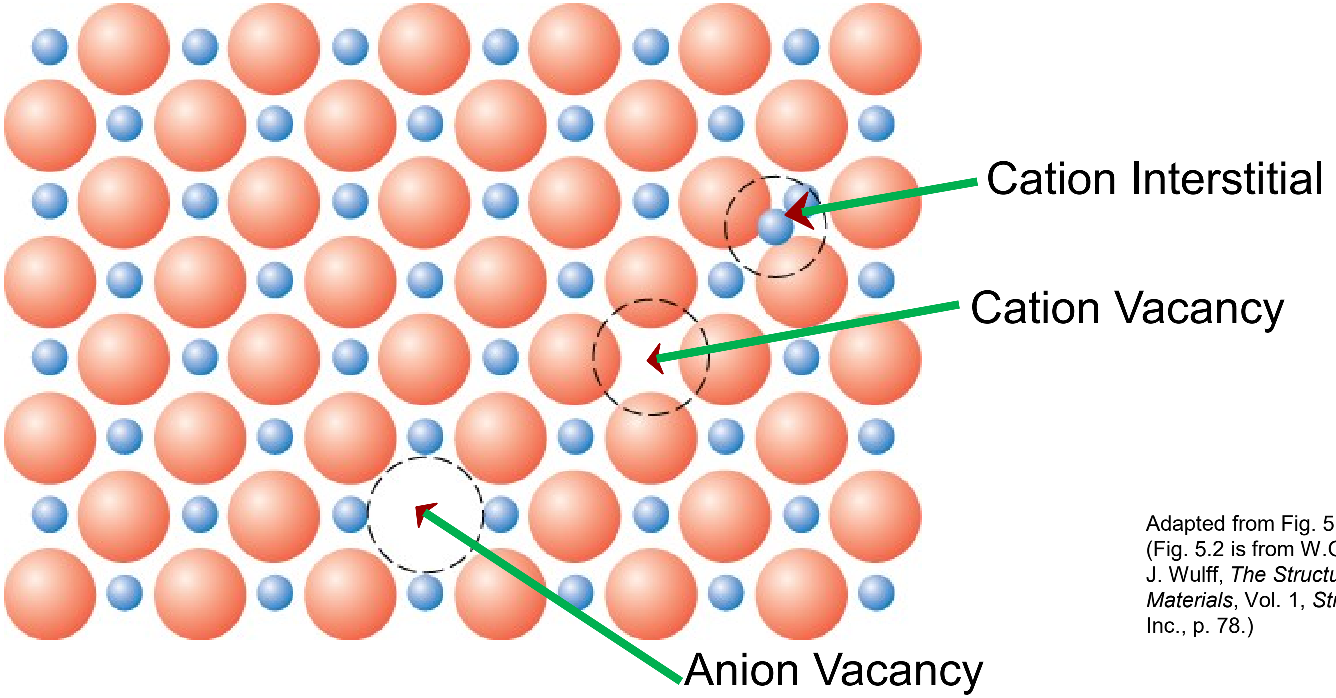
Self Interstitials



- In metals, a self interstitial introduces relatively large distortions (strain) in the surrounding lattice since the atom is substantially larger than the interstitial site.

Point Defects in Ceramics

- Vacancies
  -- vacancies exist in ceramics for both cations and anions
- Interstitials
  -- interstitials exist for cations
  -- interstitials are not normally observed for anions because anions are large relative to the interstitial sites



Adapted from Fig. 5.2, *Callister & Rethwisch 3e.* (Fig. 5.2 is from W.G. Moffatt, G.W. Pearsall, and J. Wulff, *The Structure and Properties of Materials*, Vol. 1, *Structure*, John Wiley and Sons, Inc., p. 78.)

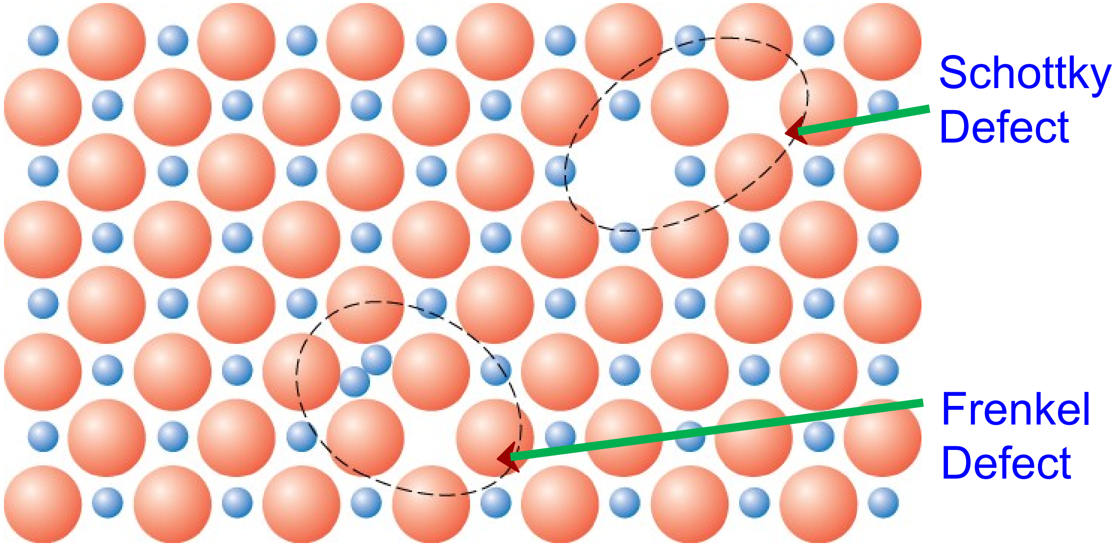
Point Defects: Frenkel and Schottky

- **Frenkel Defect**

To maintain the charge neutrality, a cation vacancy-cation interstitial pair occur together. The cation leaves its normal position and moves to the interstitial site.

- **Schottky Defect**

To maintain the charge neutrality, remove 1 cation and 1 anion; this creates 2 vacancies.



Adapted from Fig. 5.3, *Callister & Rethwisch 3e.* (Fig. 5.3 is from W.G. Moffatt, G.W. Pearsall, and J. Wulff, *The Structure and Properties of Materials*, Vol. 1, *Structure*, John Wiley and Sons, Inc., p. 78.)

Equilibrium Concentration: Point Defects

- Equilibrium concentration varies with temperature.

Activation energy –
energy required for formation of vacancy

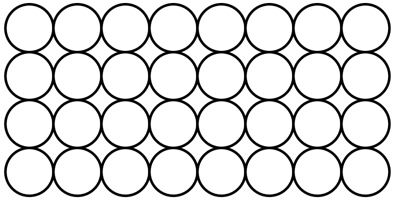
No. of defects

No. of potential defect sites

$$\frac{N_v}{N} = \exp\left(\frac{-Q_v}{kT}\right)$$

Temperature

Boltzmann's constant
(1.38×10^{-23} J/atom-K)
(8.62×10^{-5} eV/atom-K)



Each lattice site
is a potential
vacancy site

Alloying

- Given a metal (with only 1 type of atom) refined to 99.9999% purity, there would still exist 10^{22} to 10^{23} impurity atoms in 1 cubic meter of material.
- Most metals are alloys. Alloying is done to improve strength, corrosion resistance, ductility, lower melting T.
- For example, sterling silver is an alloy of 92.5% silver, 7.5% copper. At room temperature, “pure” silver is highly corrosion resistant, but also very soft. The addition of copper improves the strength and maintains good corrosion behavior.

Solid Solution

- The addition of impurity atoms to a metal results in the formation of a solid solution.
- The solvent represents the element that is present in the greatest amount (the host atoms). For example, in Lab 8 (MSE 227) Precipitation Hardening of Aluminum, aluminum is the solvent and copper is the solute (present in minor concentration).
- Solid solutions form when the solute atoms (Cu) are added to the solvent (Al), assuming the crystal structure is maintained and no new structures are formed.

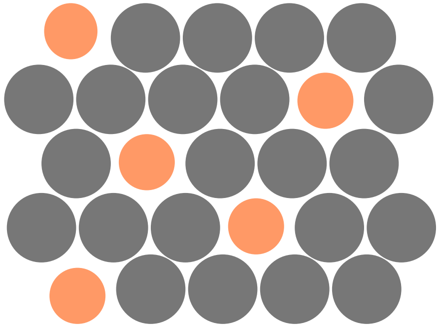
Solid Solution - continued

- A solid solution is a homogenous composition throughout.
- The impurity atoms (Cu) are randomly and uniformly dispersed within the solid.
- The impurity defects in the solid solution are either substitutional or interstitial.

Imperfections in Metals

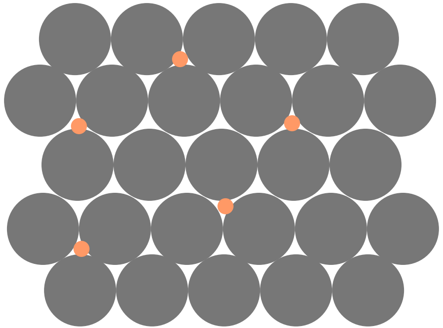
What are the outcomes if impurity (B) is added to host (A)?

- Solid solution of B in A (random distribution of point defects)



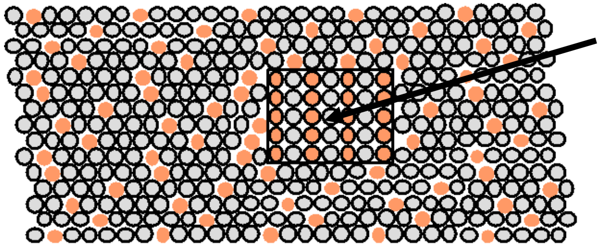
Substitutional solid solution.
(e.g., Cu in Ni)

OR



Interstitial solid solution.
(e.g., C in Fe)

- Solid solution of B in A plus particles of a new phase (usually for a larger amount of B)



Second phase particle
-- different composition
-- often different structure.

Hume - Rothery Rules

The **Hume-Rothery rules** are basic conditions for an element to dissolve in a metal, forming a substitutional solid solution.

1. The atomic radius of the solute and solvent atoms must differ by no more than 15% ($\Delta r < 15\%$).
2. The solute and solvent should have similar electronegativities.
3. Same crystal structure for “pure” metals.
4. Maximum solubility occurs when the solvent and solute have the same valence. Metals with lower valence will tend to dissolve metals with higher valence.

Substitutional Solid Solution Example: Copper and Nickel

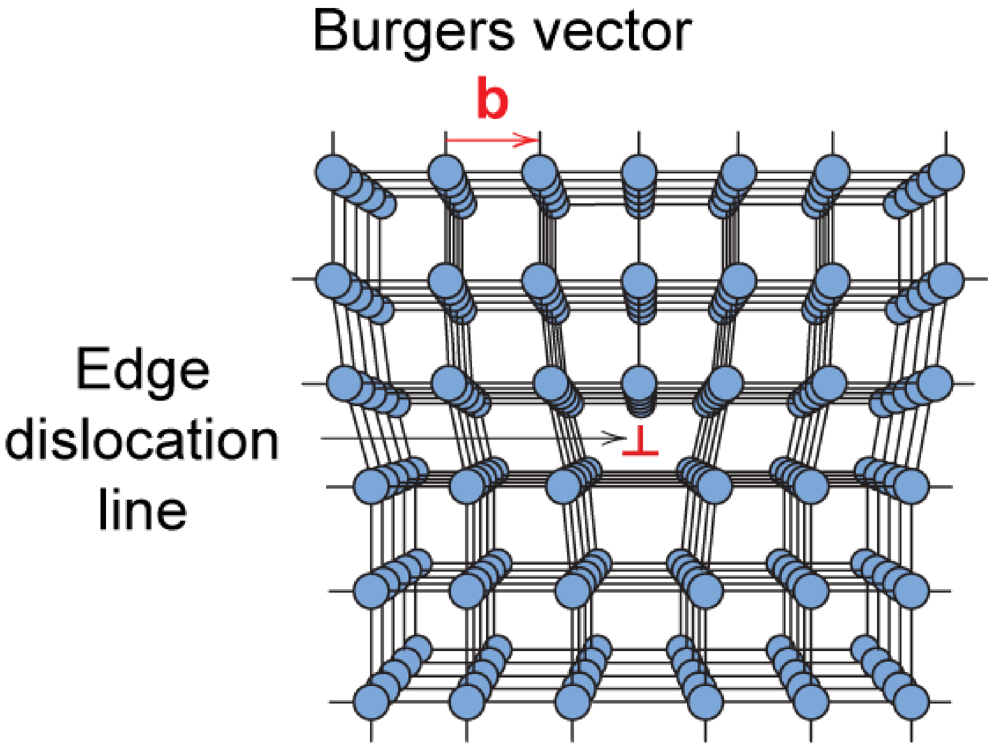
Element	*Atomic Radius (nm)*	*Crystal Structure*	*Electro-nega-tivity*	*Valence*
Cu	0.1278	FCC	1.9	+2
C	0.071		2.5	
H	0.046			
O	0.060			
Ag	0.1445	FCC	1.9	+1
Al	0.1431	FCC	1.5	+3
Co	0.1253	HCP	1.8	+2
Cr	0.1249	BCC	1.6	+3
Fe	0.1241	BCC	1.8	+2
Ni	0.1246	FCC	1.8	+2
Pd	0.1376	FCC	2.2	+2
Zn	0.1332	HCP	1.6	+2

Imperfections in Solids

Linear defects (Dislocations) are one-dimensional defects that cause misalignment of nearby atoms.

Linear defects are associated primarily with **mechanical deformation.**

Types of dislocations: edge, screw, mixed.

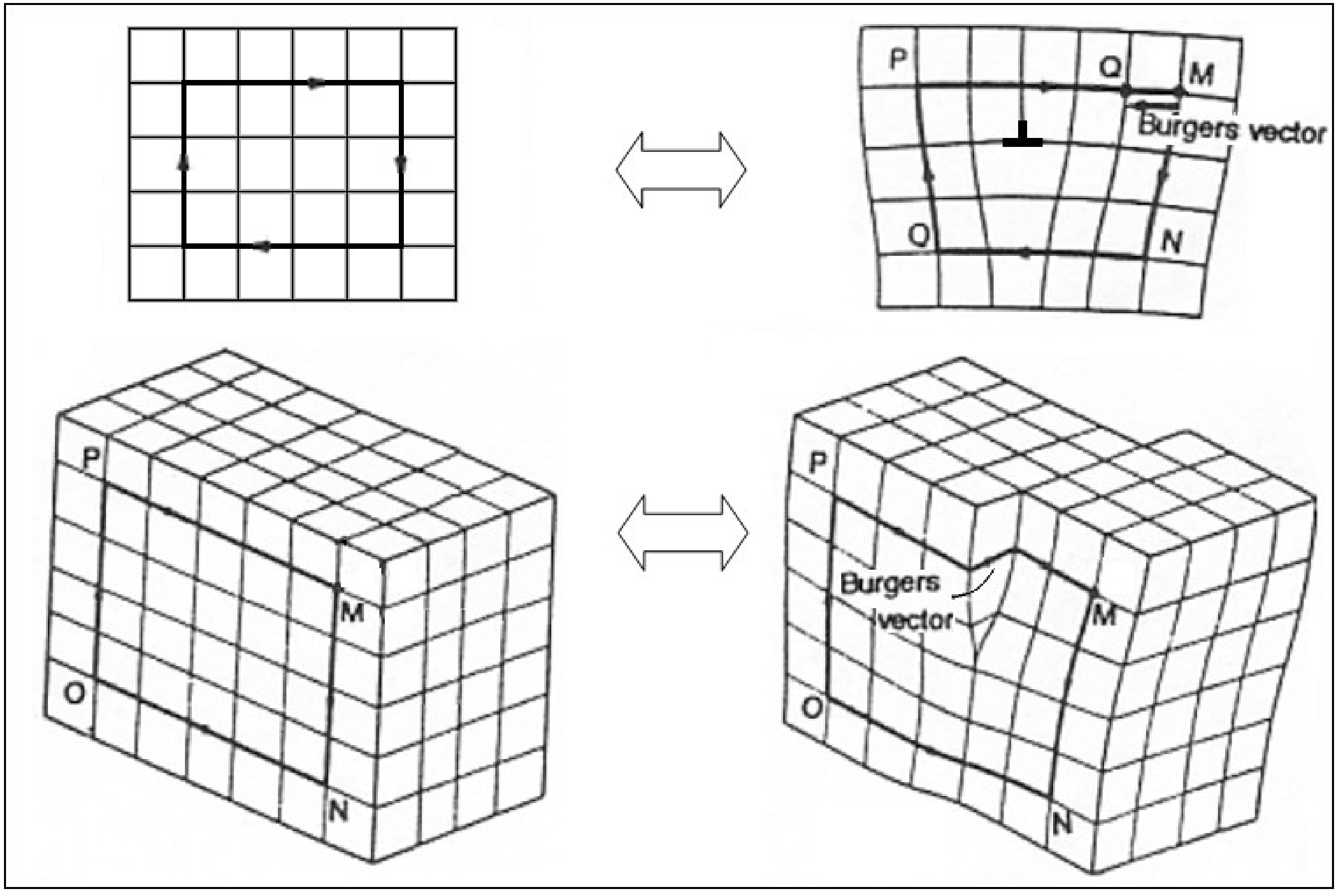


Edge dislocation:

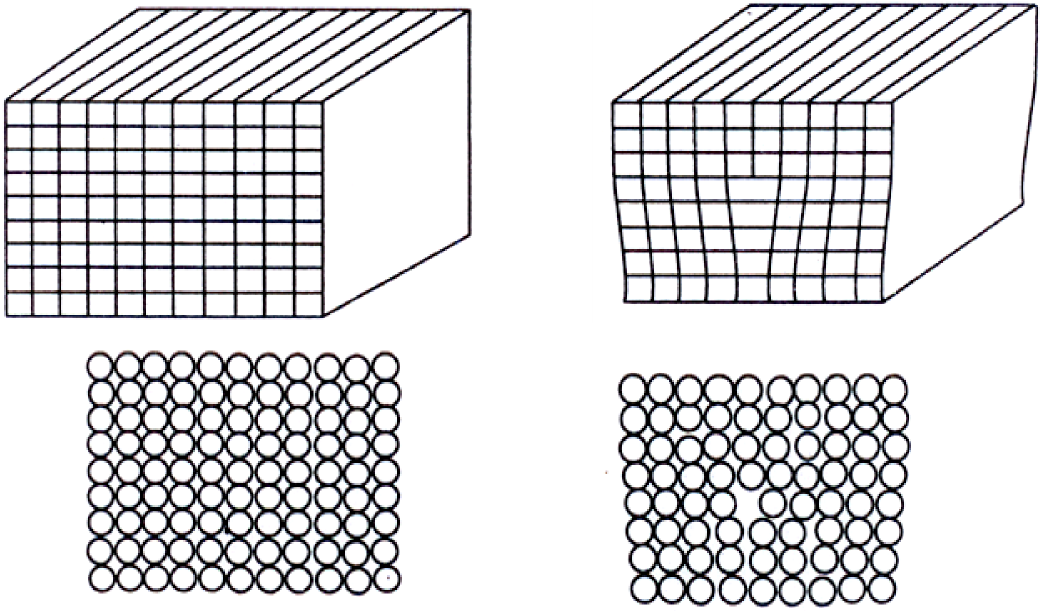
- extra half-plane of atoms inserted in a crystal structure; the edge of the plane terminates within the crystal.
- Around the dislocation line there is some localized distortion.
- **b** perpendicular (⊥) to dislocation line

Burger’s vector, **b**: measure of lattice distortion

In physics, the Burgers vector, named after Dutch physicist Jan Burgers, is a vector, often denoted b, that represents the magnitude and direction of the lattice distortion resulting from a dislocation in a crystal lattice



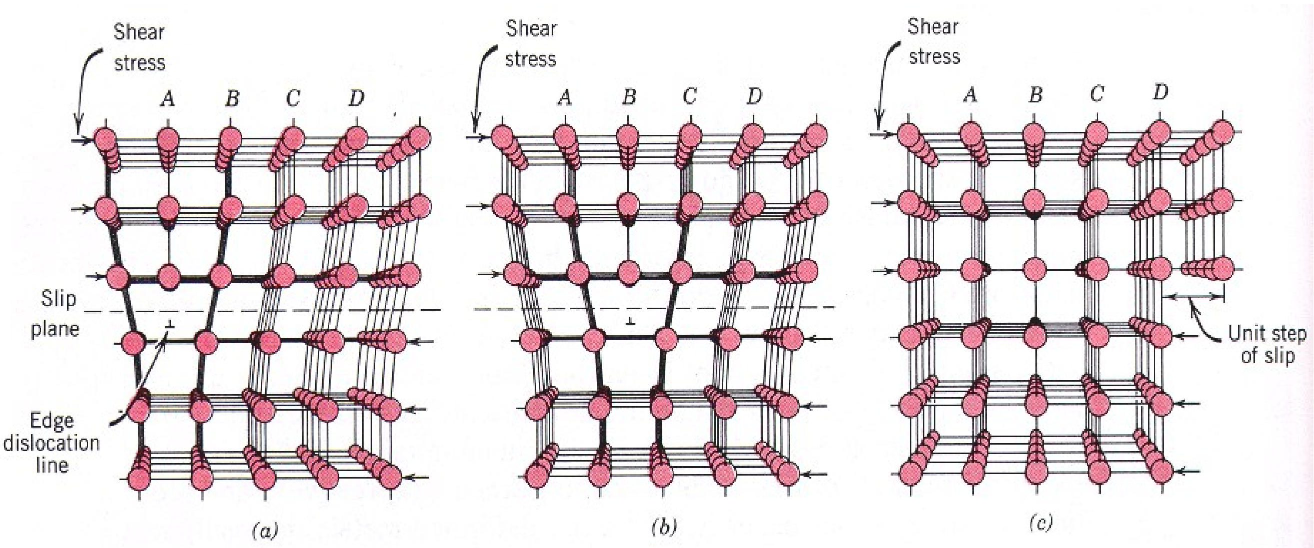
EDGE DISLOCATION



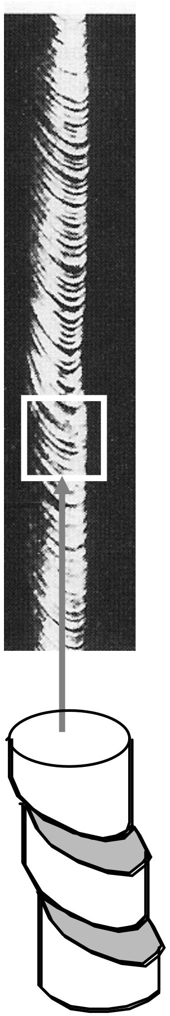
(a) (b)

Dislocation Motion

- Produces plastic deformation,
- Depends on incrementally breaking bonds.



- If dislocations don't move, deformation doesn't happen!



Plastically stretched zinc single crystal.

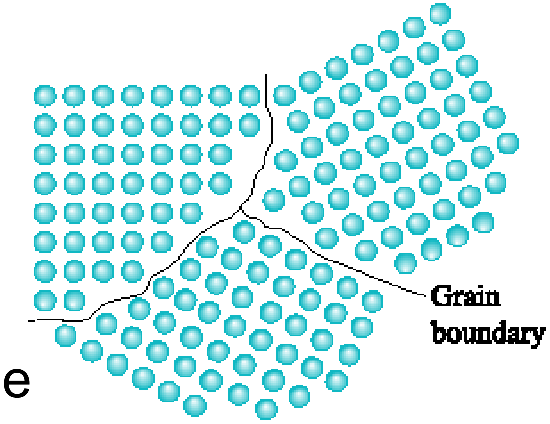
Polycrystalline Materials

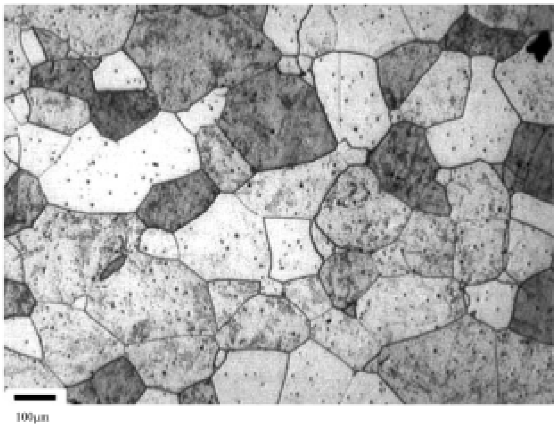
Grain Boundaries

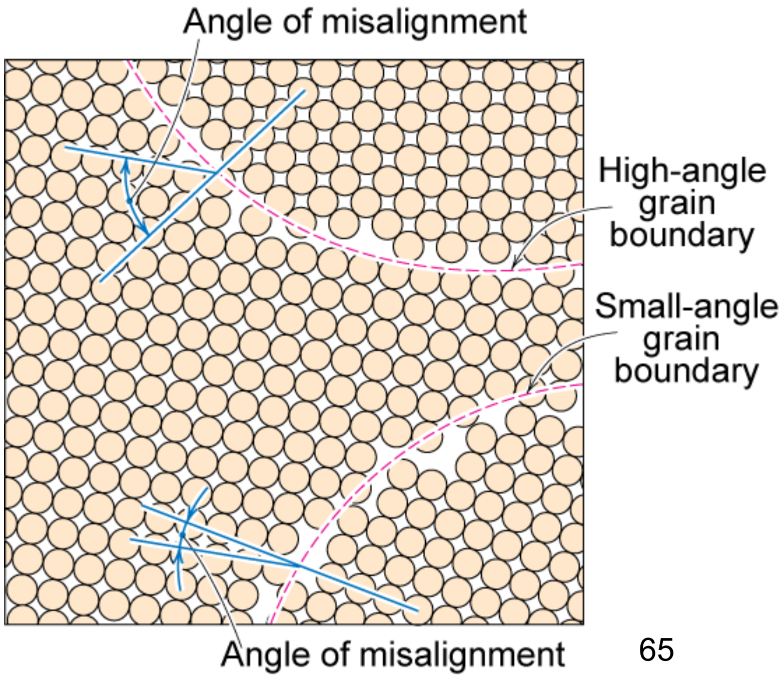
- regions between crystals
- transition from lattice of one region to another

(a) The atoms near the boundaries of the 3 grains do not have an equilibrium spacing or arrangement; slightly disordered.

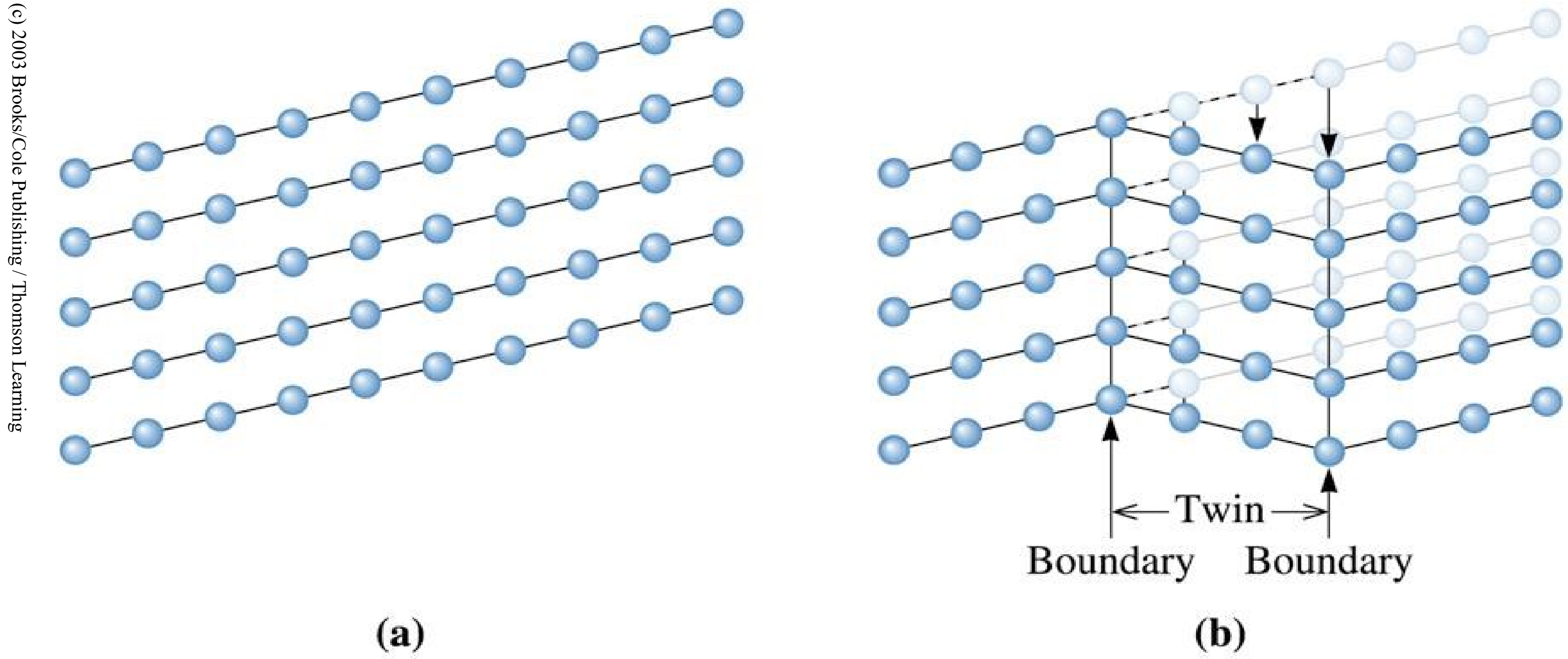
(b) Grains and grain boundaries in a stainless steel sample. low density in grain boundaries





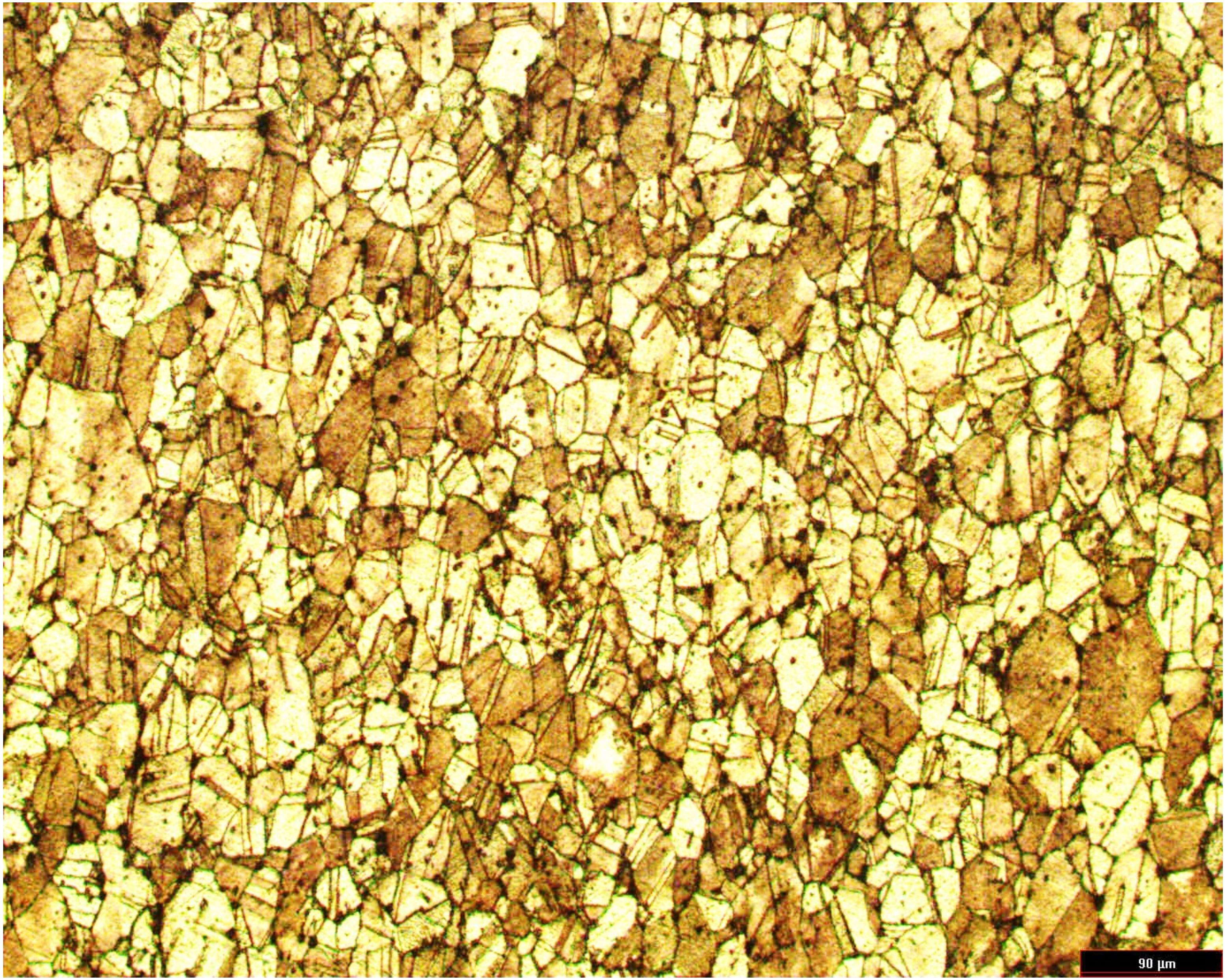


Twinning



Applied stress to a perfect crystal (a) may cause a displacement of the atoms, (b) causing the formation of a twin. Note that the crystal has deformed as a result of twinning.

Brass (90 micron scale bar)



STACKING FAULTS

- Whenever the stacking of atomic planes is not in a proper sequence throughout the crystal, the fault caused is known as ***stacking fault***.
- For example, the stacking sequence in an ideal FCC crystal may be described as A-B-C-A-B-C- A-B-C-……. But the stacking fault may change the sequence to A-B-C-A-B-A-B-A-B-C. The region in which the stacking fault occurs (A-B-A-B) forms a thin region and it becomes HCP.
- This thin region is a surface imperfection and is called a stacking fault.