BFF1113
Engineering Materials

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Course Guidelines:

1. Introduction to Engineering Materials
2. Bonding and Properties
3. Crystal Structures & Properties
4. Imperfection in Solids
5. Mechanical Properties of Materials
6. Physical Properties of Materials
7. Failure & Fundamental of Failure
8. Metal Alloys
9. Phase Diagram
10. Phase Transformation – Heat Treatment
11. Processing and Application of Metals
12. Ceramic Materials
13. Polymer Materials
14. Composite Materials
15. Corrosion & Degradation of Materials
16. Environment and Sustainability

Bonding and Properties

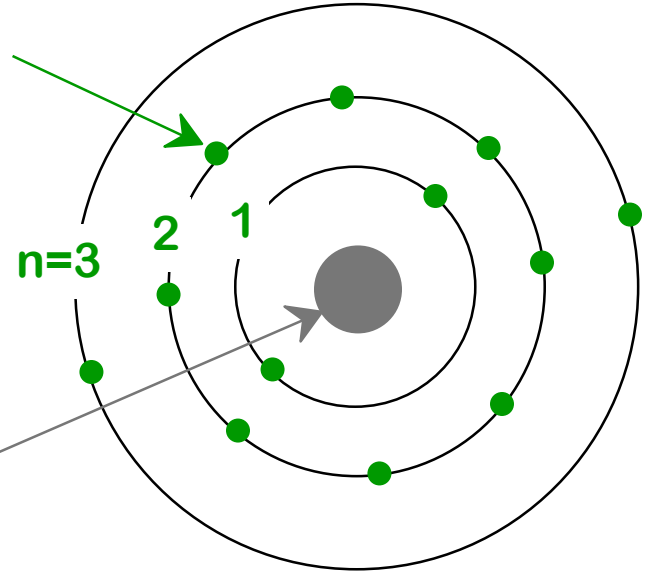
1. Atomic structure and bonding
2. Crystal structures and properties
3. Crystalline and non-crystalline materials
4. Imperfection in solids

ATOMIC MODELS

Simplified Atomic Model

Some Terminologies (basic structure for elements)

orbital electrons:



ATOM

Very small nucleus composed of protons & neutrons which is encircled by moving electrons

- **Nucleus (Proton + Neutron)**

$$^{A}_{Z}X$$

A → Atomic Mass

Z → Atomic Number

Atomic mass (A) ≈ Z + N

- Z (atomic number) = # protons
- N = # neutrons

<u>Example:</u>

Determine the number of Proton, electron and neutron in a fluorine atom.

<u>Answer:</u>

A = p + n = 19

Z = p = e = 9

➔ n = A – Z = 19 – 9 = 10

- Proton = 9
- Electron = 9
- Neutron = 10

$$^{19}_{9}F$$

The mass and charge of Proton, Neutron, and Electron

	Mass (g)	Charge (C)
Proton	1.673×10^{-24}	$+1.602 \times 10^{-19}$
Neutron	1.675×10^{-24}	0
Electron	9.109×10^{-28}	-1.602×10^{-19}

1. INTERATOMIC BONDING

Why we need to understand the concept of interatomic bonding in solids?

Some important properties of solid depend on geometrical atomic arrangements & also the interactions that exist among constituent atoms or molecules

Example: Carbon ~ graphite & diamond

Interatomic Bonding

Primary Bonding

- Ionic bonds
- Covalent bonds
- Metallic bonds

Secondary Bonding

- Van der Waals bonds
- Hydrogen bond

- 3 different types of **primary** or chemical bond are found in solids.
  - **Ionic, covalent, and metallic**.
  - Involve valence electrons
  - Nature of bond depends on electron structures of the constituent atoms.

    Tendency of atoms to assume stable electron structure.
- **Secondary** (or physical) forces and energies also found in many solid materials.
  - **Wan Der Waals, Hydrogen bond**
  - Weaker than primary ones
  - Influence physical properties of some material

1.1: Primary Interatomic Bonds

- Primary Bonding
  - > Ionic Bonding
  - > Covalent Bonding
  - > Metallic Bonding

Ionic Bonding

- Formed between highly electropositive (metallic) elements and highly electronegative (nonmetallic) elements.
- Ionization: electrons are transferred from atoms of electropositive elements to atoms of electronegative elements, producing positively charged cations and negatively charge anions.
- Ionic bonding: due to **electrostatic / coulombic force** attraction of oppositely charged ions.
- Binding energy ➔ large ➔ high melting temp.
- Ionic material ➔ hard, brittle, electrically and thermally insulative.

EXAMPLES: IONIC BONDING

- **Predominant bonding in Ceramics**

NaCl

MgO

CaF_2

CsCl

IA																	0
H 2.1	IIA										IIIA	IVA	VA	VIA	VIIA		He -
Li 1.0	Be 1.5										5 B 2.0	6 C 2.5	7 N 3.0	O 3.5	F 4.0		Ne -
Na 0.9	Mg 1.2	IIIB	IVB	VB	VIB	VIIB	VIII			IB	IIB	13 Al 1.5	14 Si 1.8	15 P 2.1	16 S 2.5	Cl 3.0	Ar -
K 0.8	Ca 1.0	21 Sc 1.3	Ti 1.5	23 V 1.6	Cr 1.6	25 Mn 1.5	Fe 1.8	27 Co 1.8	Ni 1.8	29 Cu 1.9	Zn 1.8	31 Ga 1.6	32 Ge 1.8	As 2.0	34 Se 2.4	Br 2.8	Kr -
Rb 0.8	Sr 1.0	39 Y 1.2	40 Zr 1.4	41 Nb 1.6	42 Mo 1.8	43 Tc 1.9	44 Ru 2.2	45 Rh 2.2	46 Pd 2.2	47 Ag 1.9	48 Cd 1.7	49 In 1.7	50 Sn 1.8	51 Sb 1.9	52 Te 2.1	I 2.5	Xe -
Cs 0.7	Ba 0.9	57–71 La–Lu 1.1–1.2	72 Hf 1.3	73 Ta 1.5	74 W 1.7	75 Re 1.9	76 Os 2.2	77 Ir 2.2	78 Pt 2.2	79 Au 2.4	80 Hg 1.9	81 Tl 1.8	82 Pb 1.8	83 Bi 1.9	84 Po 2.0	At 2.2	Rn -
Fr 0.7	Ra 0.9	89–103 Ac–No 1.1–1.7															

Give up electrons (electropositive)

Acquire electrons (electronegative)

Adapted from Fig. 2.7, *Callister 6e.* (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.

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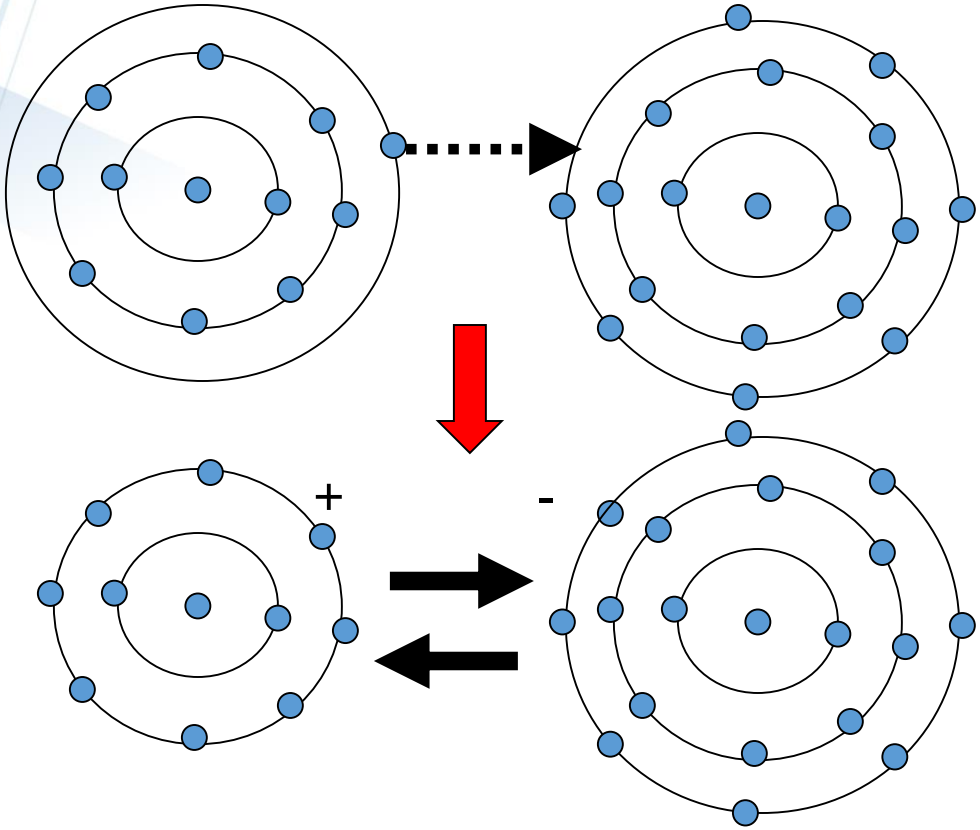
Unstable

Unstable

Sodium atom, Na

Chlorine atom, Cl



Sodium ion, Na^+

Chlorine ion, Cl^-

Stable

Stable

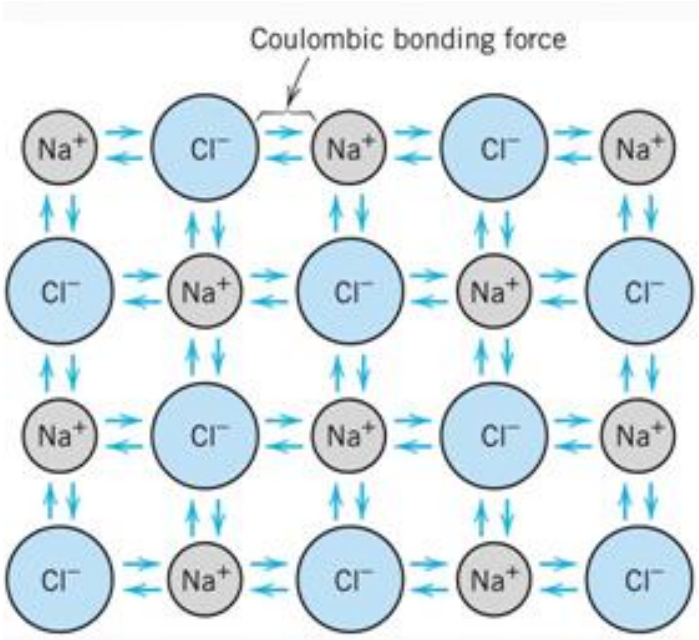


FIGURE 2.9 Schematic representation of ionic bonding in sodium chloride (NaCl).

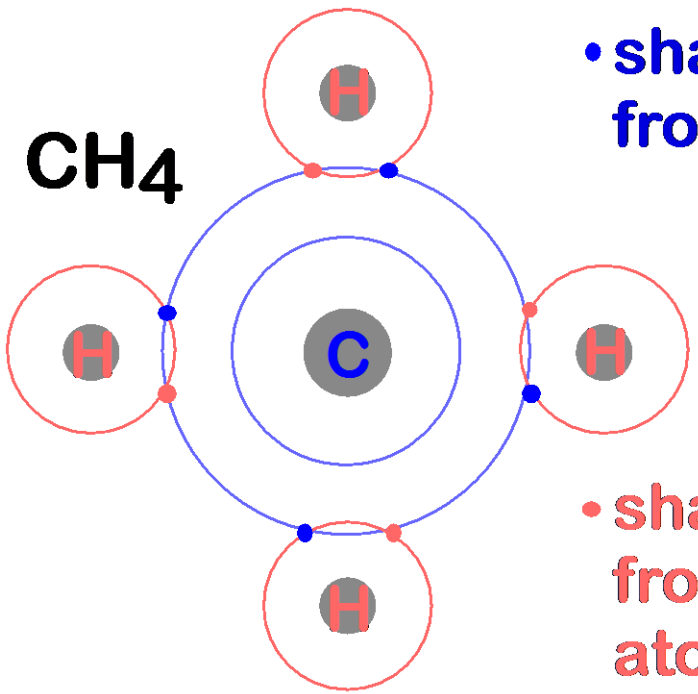
Covalent Bonding

- In covalent bonding stable electron configurations are assumed by sharing of electrons between adjacent atoms.
- Two atoms that are covalently bonded will each contribute at least one electron to the bond, and the shared electrons may be considered to belong to both atoms.
- H• + H• $\rightarrow$ H:H (1s^1 electron from hydrogen atom)
- Many nonmetallic elemental molecules (H_2, Cl_2, F_2, etc)
- Molecules containing dissimilar atoms (CH_4, H_2O, HNO_3, HF, etc)
- Other elemental solids: diamond (carbon), silicon, germanium
- Binding energy & melting temp for covalently bonded materials ➔ very high (diamond) to very weak (bismuth, polymeric material)
- Possible of having interatomic bonds (partially ionic and partially covalent).

- **Example: CH_4 (methane)**

C: has 4 valence e, needs 4 more

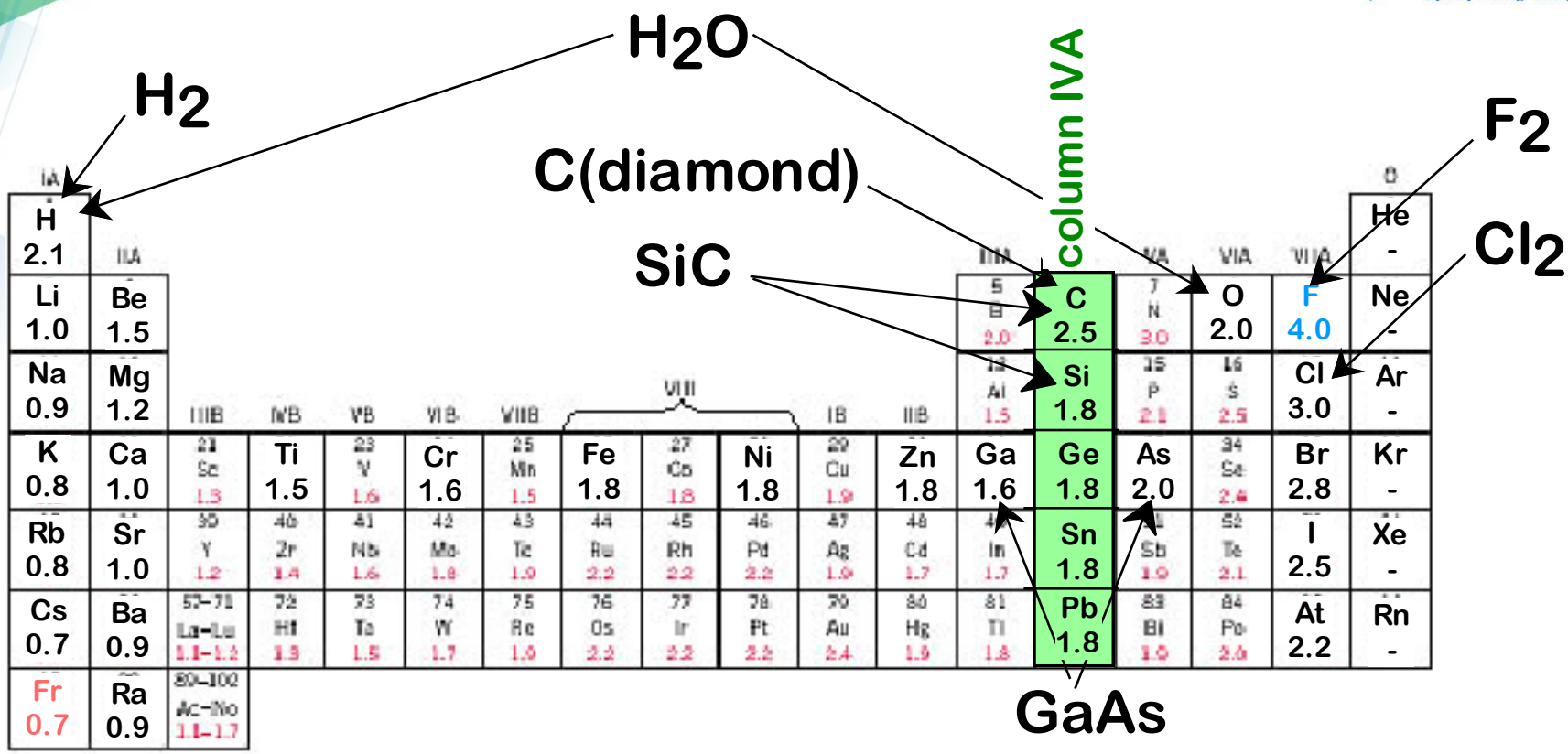
H: has 1 valence e, needs 1 more



- **shared electrons from carbon atom**

- **shared electrons from hydrogen atoms**

EXAMPLES: COVALENT BONDING



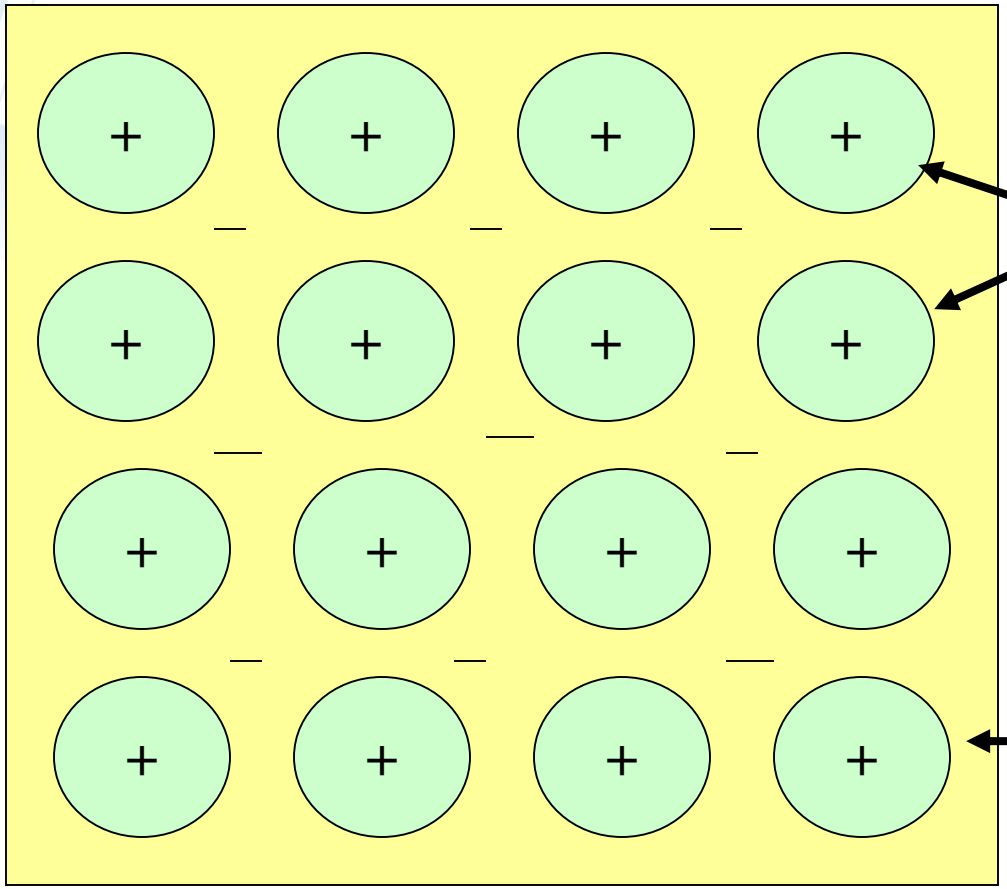
- Molecules with nonmetals
- Molecules with dissimilar atoms
- Elemental solids (RHS of Periodic Table)
- Compound solids (about column IVA) (SiC, GaAs)

Adapted from Fig. 2.7, *Callister 6e.* (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.

Metallic Bonding

- Very similar to covalent bonding
- Valence electrons
  - Metallic materials have 1, 2, or 3 valence electrons.
  - not bound to any particular atom in the solid.
  - are essentially free electrons and move (drift) through out the metal.
  - form a **sea of electron or electron cloud.**
- Remaining non-valence electrons and atomic nuclei ➔ ion cores
- Group IA and IIA elements
- All elemental metals
- Highly conductive
- Ductile,
- Binding energy & melting temp (wide range)

Schematic illustration of metallic bonding



Ion cores

- nonvalence electrons and atomic nuclei

-posses a net positive charge equal in magnitude to the total valence electron charge per atom.

Sea of valence electrons

- The free electrons shield the positively charged ion chores from electrostatic forces.
- This free electrons act as a “glue” to hold the ion cores together.

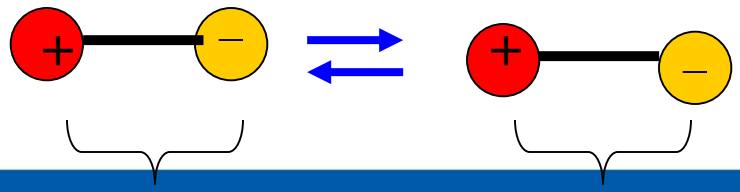
1.2: Secondary Bonds

Van der Waals Bonds

- Van der Waals bond or physical bond
- Binding energy (typical) ➔ in the order of 10 kJ/mol (0.1 eV/atom)
- Exist between virtually all atoms or molecules.
- The presence of any of the 3 primary bonding types may obscure it.
- The driving force for secondary bonding is the attraction of the electric dipoles contained in atoms or molecules
- Electric dipoles:

- separation of positive and negative portions of an atom or molecule. - coulombic attraction between +ve end of one dipole and –ve end dipole.

Schematic illustration of van der Waals bonding between two dipoles



Atomic or molecular dipoles

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Bonding Energies and Melting Temperatures for Various Substances

Bonding Type	Substance	Bonding Energy		Melting Temperature (°C)
		kJ/mol	eV/atom, ion, molecule	
Ionic	NaCl	640	3.3	801
	MgO	1000	5.2	2800
Covelent	Si	450	4.7	1410
	C (diamond)	713	7.4	>3550
Metallic	Hg	68	0.7	-39
	Al	324	3.4	660
	Fe	406	4.2	1538
	W	849	8.8	3410
Van der Waals	Ar	7.7	0.08	-189
	Cl_2	31	0.32	-101
Hydrogen	NH_3	35	0.36	-78
	H_2O	51	0.52	0

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READ….

HYDROGEN BONDS

THINK….

WHY ICE CUBES FLOAT IN WATER

2.0 Crystal Structures & Properties

3.0 Crystalline and non-crystalline materials

- Introduction
- Arrangement of atom in metallic crystal structures
- Single crystal, polycrystalline materials
- X-ray diffraction: determination of crystal structure

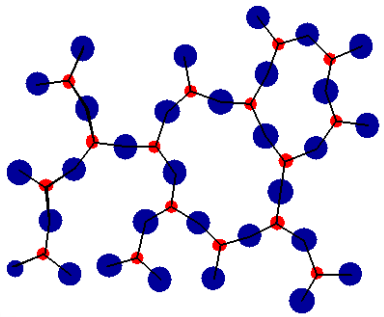
At the end of the lecture, students will be able:

1. To describe the difference in atomic/molecular structure between crystalline and noncrystalline materials.
2. To draw unit cells for face-centered cubic (FCC), body-centered cubic (BCC), and hexagonal close-packed crystal (HCP) structures.
3. To derive the relationships between unit cell edge length and atomic radius for FCC and BCC crystal structures.
4. To compute the densities for metals having FCC and BCC crystal structures given their unit cell dimensions.
5. To distinguish between single crystals and polycrystalline materials.
6. To describe briefly the use of XRD to identify an element.

ARRANGEMENT OF ATOMS

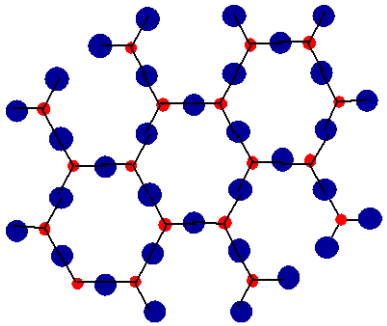
- Solid materials:
  - Classified according to the regularity with which atoms or ions are arranged with respect to one another.
- 2 types:
  - Crystalline materials
  - Noncrystalline (or amorphous) materials

Noncrystalline vs. crystalline SiO_2



noncrystalline SiO_2

• Si • Oxygen



crystalline SiO_2

Noncrystalline materials...

- atoms have no periodic or repeating packing (not systematic).
- has no long range atomic order.

occurs for: -complex structures, -rapid cooling

"Amorphous" = Noncrystalline

Crystalline materials...

- atoms pack in periodic (or repeating), over large atomic distances (long range order)
- typical of: -metals, -many ceramics, -some polymers

Note: There is an extremely large number of different crystal structures all having long range atomic order, depending how you ARRANGE and PACK it.

How many types of crystal structures are available?

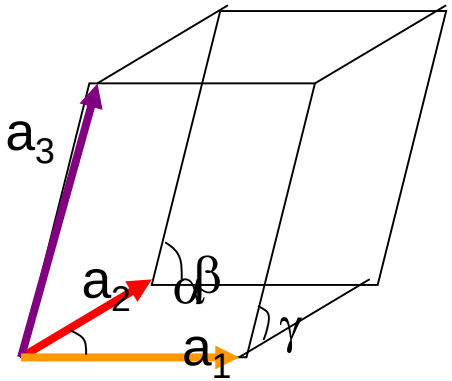
- How many types of unit cell? (Unit cell – small repeat entities)

  ***Smallest group of atoms showing the **lattice structure** is known as a **unit cell**

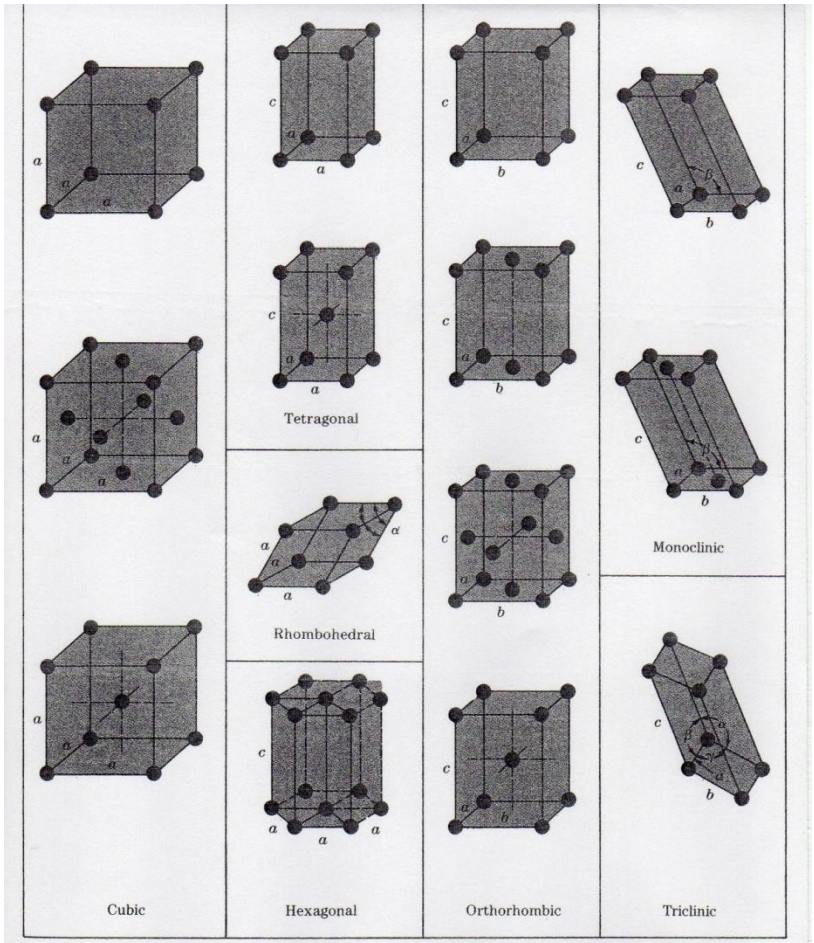
- Depends on types of lattices (3D array of point coinciding with atom positions)

- There is an unlimited number of possible lattices because there is no natural restriction on the <u>lengths of lattice translation vectors</u> or on the <u>angle φ</u> between them.

- 3 primary directional length + 3 angles between the 3 directions ➔ type of unit cell



Crystal system	Restriction on conventional cell axes and angles
Triclinic	$a_1 \neq a_2 \neq a_3$ $\alpha \neq \beta \neq \gamma$
Monoclinic	$a_1 \neq a_2 \neq a_3$ $\alpha = \gamma = 90^o \neq \beta$
Orthorhombic	$a_1 \neq a_2 \neq a_3$ $\alpha = \gamma = \beta = 90^o$
Tetragonal	$a_1 = a_2 \neq a_3$ $\alpha = \gamma = \beta = 90^o$
Cubic	$a_1 = a_2 = a_3$ $\alpha = \gamma = \beta = 90^o$
Trigonal	$a_1 = a_2 = a_3$ $\alpha = \beta = \gamma < 120^o, \neq 90^o$
Hexagonal	$a_1 = a_2 \neq a_3$ $\alpha = \beta = 90^o$ $\gamma = 120^o$



IGURE 3.2 The 14 Bravais conventional unit cells grouped according to crystal system. The dots indicate attice points that, when located on faces or at corners, are shared by other identical lattice unit cells. After W. G. Moffatt, G. W. Pearsall, and J. Wulff, "The Structure and Properties of Materials," vol. I: Structure," Wiley, 1964, p. 47.)

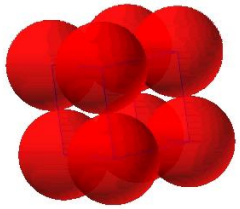
The Crystal Structure of Metals

- have the simplest crystal structures.

3 basic atomic arrangements:

1. **Face-centered cubic (fcc)**
2. **Body-centered cubic (bcc)**
3. **Hexagonal close-packed (hcp)**

FYI only: SIMPLE CUBIC STRUCTURE (SC)



- Rare due to poor packing (only Polonium has this structure)
- Close-packed directions at cube edges (1 unit cell).

- Assumptions used to describe crystal structure:
  - When describing crystalline structures, atoms (or ions) are thought of as being solid spheres having well defines diameters (2 R).
  - This is termed the atomic hard sphere model in which spheres representing nearest-neighbor atoms touch one another.

FACE CENTERED CUBIC STRUCTURE (FCC)

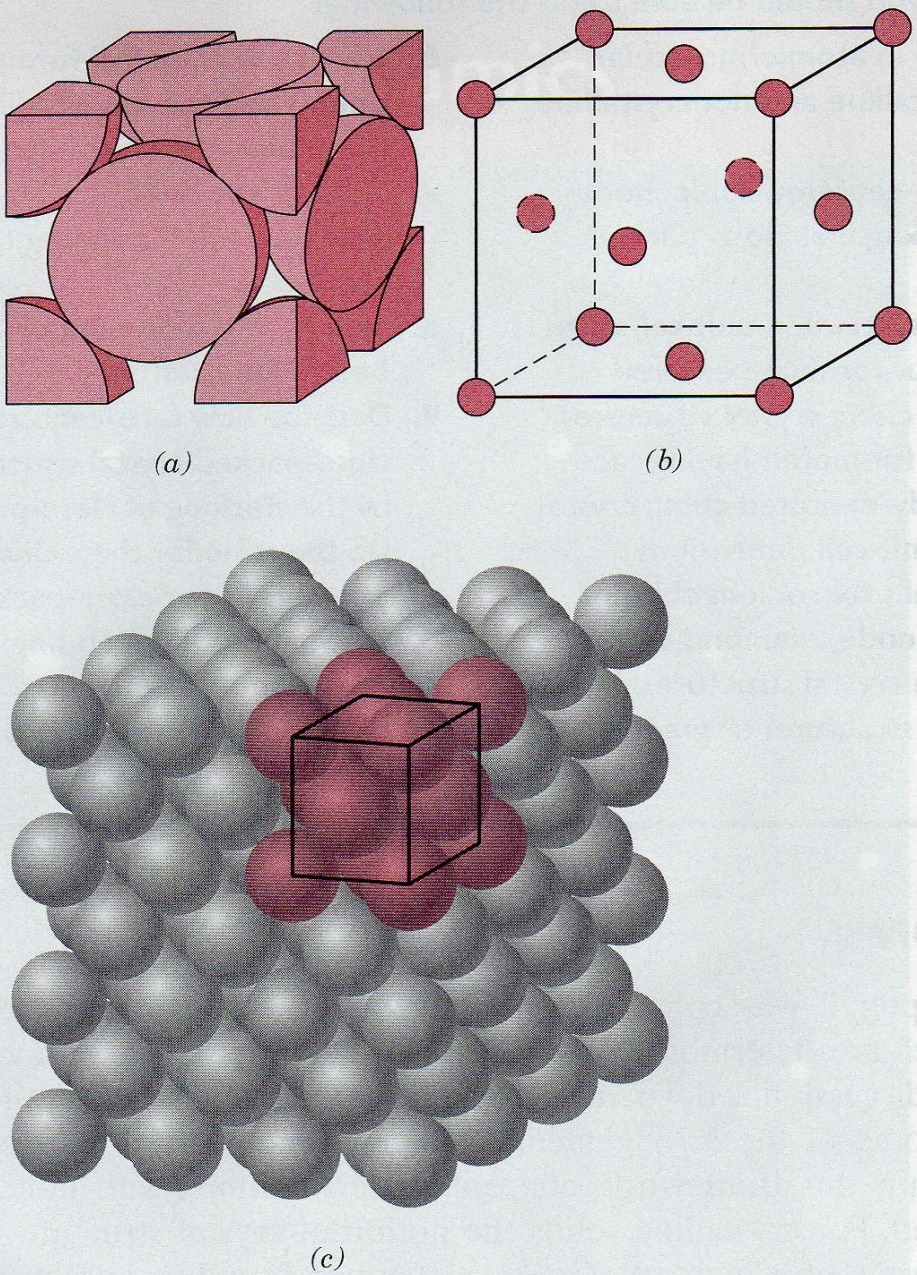
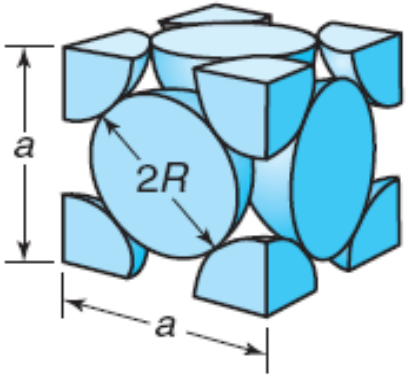
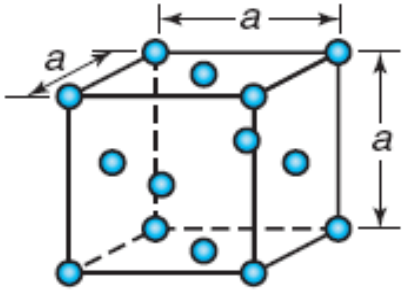


Figure 3.1 For the face-centered cubic crystal structure: (*a*) a hard sphere unit cell representation, (*b*) a reduced-sphere unit cell, and (*c*) an aggregate of many atoms. (Figure (*c*) adapted from W. G. Moffatt, G. W. Pearsall, and J. Wulff, *The Structure and Properties of Materials,* Vol. I,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

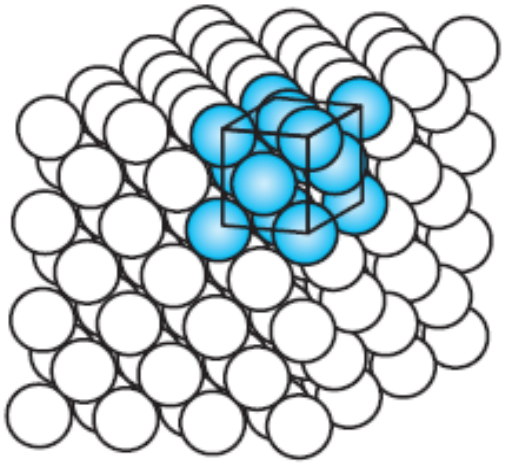
6 atom locate at surface (shared), 8 at corners (shared).



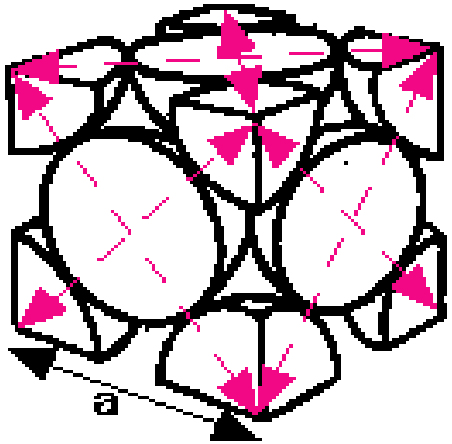
Hard-ball model



Unit cell



Single crystal with many unit cells



Equivalent number of atom

= 6 x 1/2 + 1/8 x 8

= 4 atom/unit

a = the cube edge length

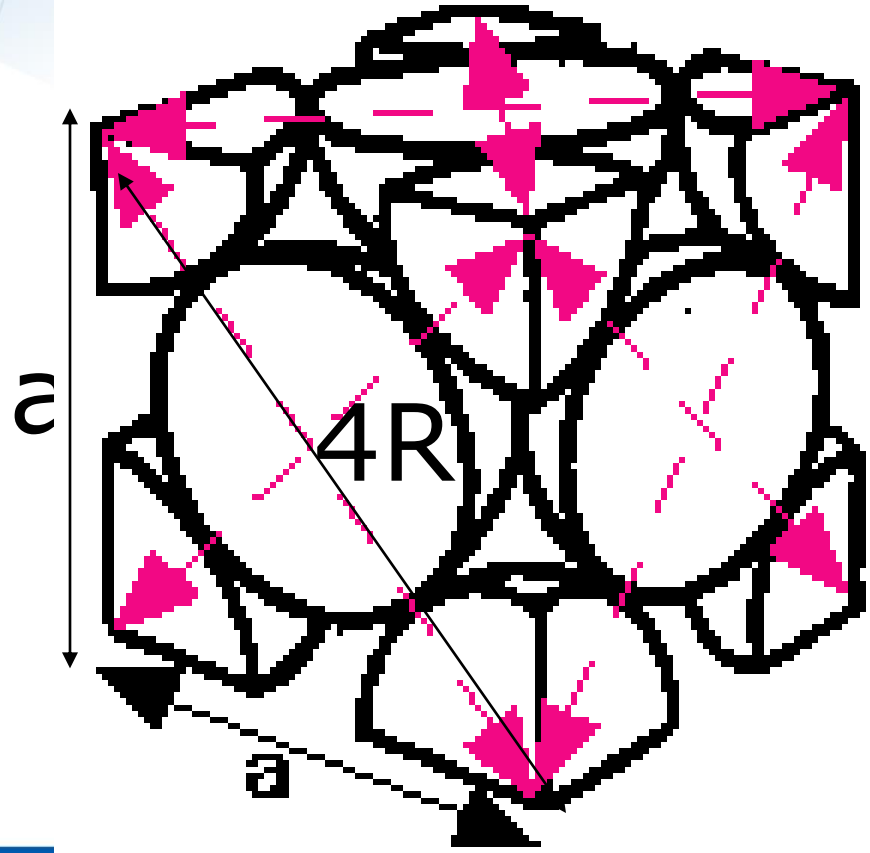
CALCULATIONS:

1)VOLUME OF CELL

2)ATOMIC PACKING FACTOR

Example 1:

Calculate the volume of a FCC cell with atomic radius of R.



$$a^2 + a^2 = (4R)^2$$

$$a = 4R/\sqrt{2}$$

$$\text{Volume} = a^3$$

$$= (4R/\sqrt{2})^3$$

Volume = Width x Length x Height

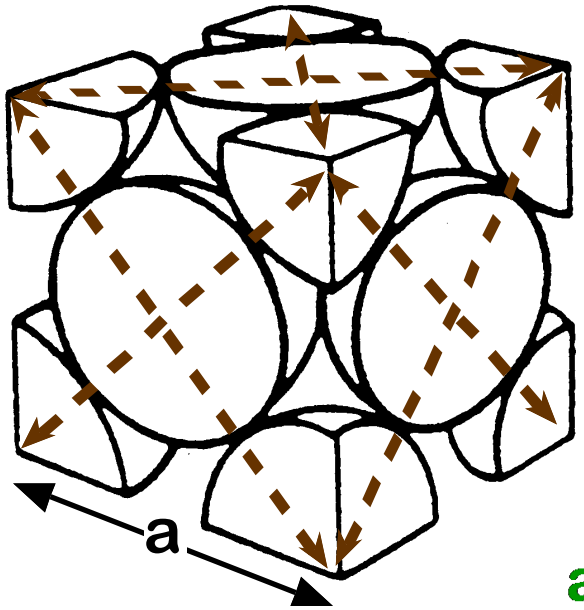
ATOMIC PACKING FACTOR
(Fraction of spaced occupied by atoms)

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

*assume hard spheres

ATOMIC PACKING FACTOR: FCC

- APF for a face-centered cubic structure = 0.74



Close-packed directions:

length = 4R

$= \sqrt{2}\, a$

Unit cell contains:

6 x 1/2 + 8 x 1/8

= 4 atoms/unit cell

$$APF = \frac{\overset{\text{atoms}}{\text{unit cell}} \; 4 \; \overset{\text{volume}}{\text{atom}} \; \frac{4}{3}\pi(\sqrt{2}a/4)^3}{\underset{\text{volume}}{\text{unit cell}} \; a^3}$$

Example 2:

Prove that the APF of FCC = 0.74, in term of the atomic radius, R:

APF = V atom/ V unit cell

V atom = $(4)(4/3\pi R^3) = 16.757R^3$

V unit cell = a^3

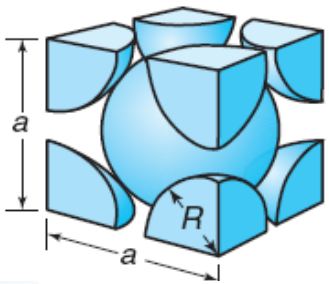
$= (4R/\sqrt{2})^3$

$= 22.63R^3$

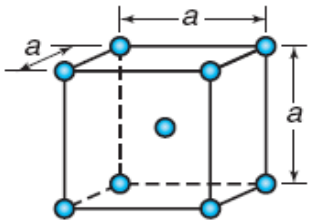
APF = $16.757R^3 / 22.63R^3$

= 0.74

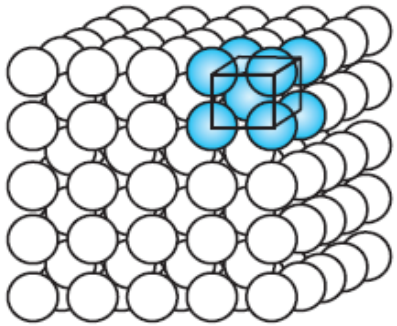
BODY CENTERED CUBIC STRUCTURE (BCC)



Hard-ball model



Unit cell



Single crystal with many unit cells

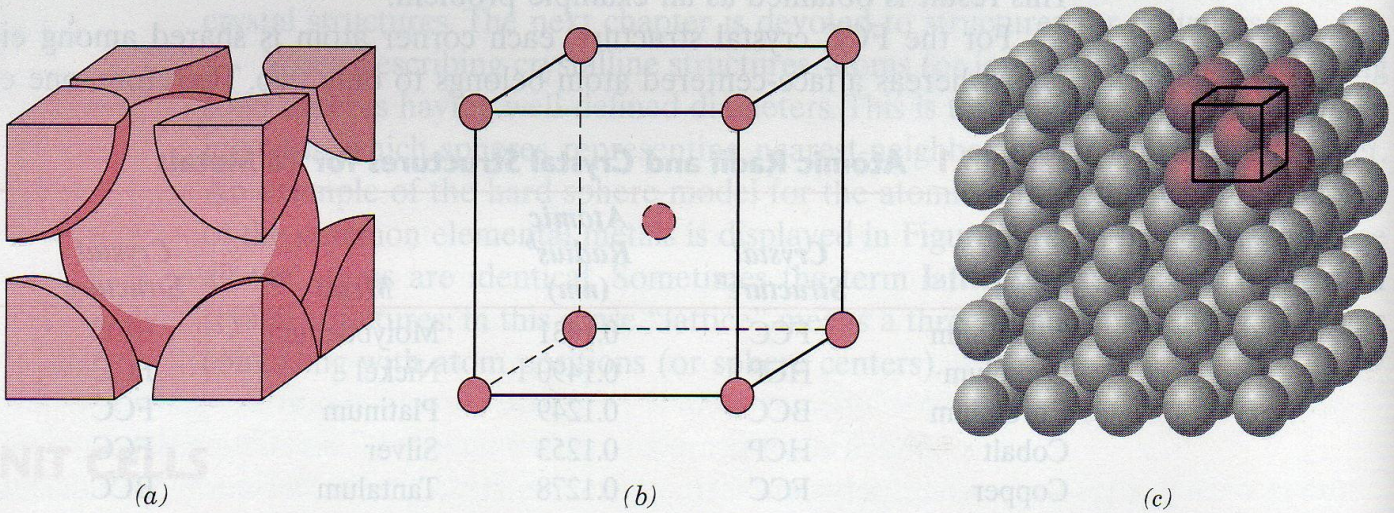
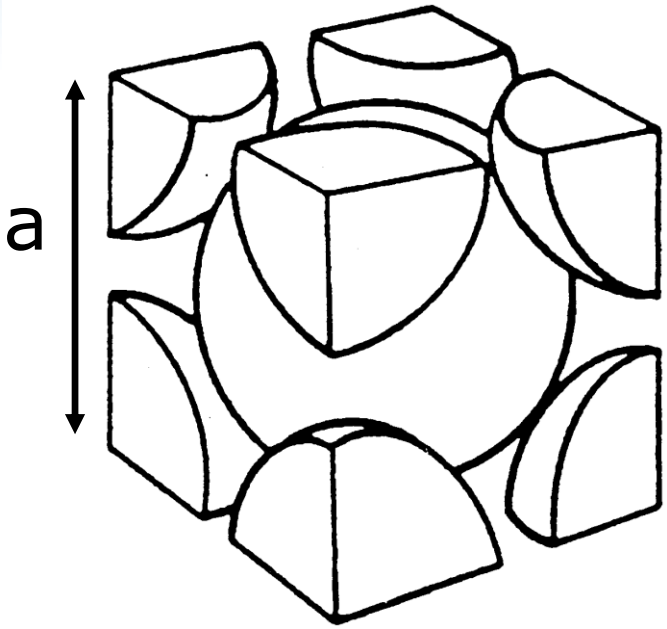


Figure 3.2 For the body-centered cubic crystal structure, (*a*) a hard sphere unit cell representation, (*b*) a reduced-sphere unit cell, and (*c*) an aggregate of many atoms. (Figure (*c*) from W. G. Moffatt, G. W. Pearsall, and J. Wulff, *The Structure and Properties of Materials,* Vol. I, *Structure,* p. 51. Copyright © 1964 by John Wiley & Sons, New York. Reprinted by permission of John Wiley & Sons, Inc.)

- **1 atom locate at center, 8 at corners (shared)**

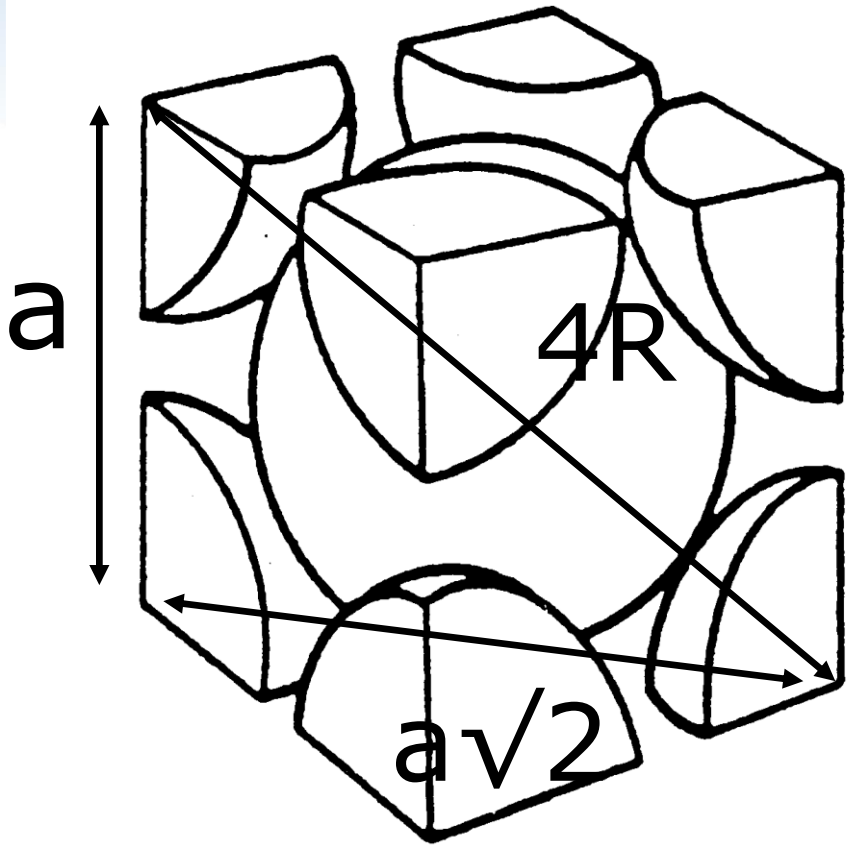
CLASS ACTIVITY !!



Calculate the volume of a BCC cell with atomic radius of R.

Example 2:

Calculate the volume of a BCC cell with atomic radius of R.



$$a^2 + (a\sqrt{2})^2 = (4R)^2$$

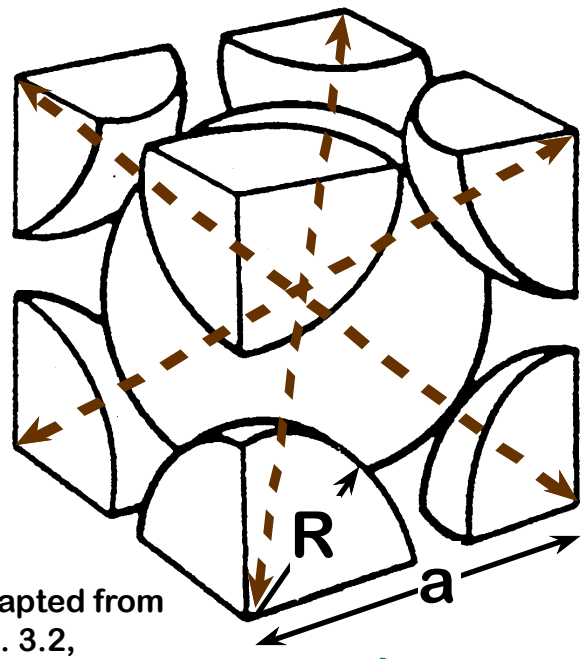
$$a = 4R/\sqrt{3}$$

$$\text{Volume} = a^3$$

$$= (4R/\sqrt{3})^3$$

ATOMIC PACKING FACTOR: BCC

- APF for a body-centered cubic structure = 0.68



Adapted from Fig. 3.2, *Callister 6e.*

Close-packed directions:

length = 4R

$= \sqrt{3}\,a$

Unit cell contains:

1 + 8 x 1/8

= 2 atoms/unit cell

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

Example 3:

Prove the APF of BCC = 0.68

APF = V atom/ V unit cell

V atom = $(2)(4/3\pi R^3) = 8.373R^3$

V unit cell = a^3

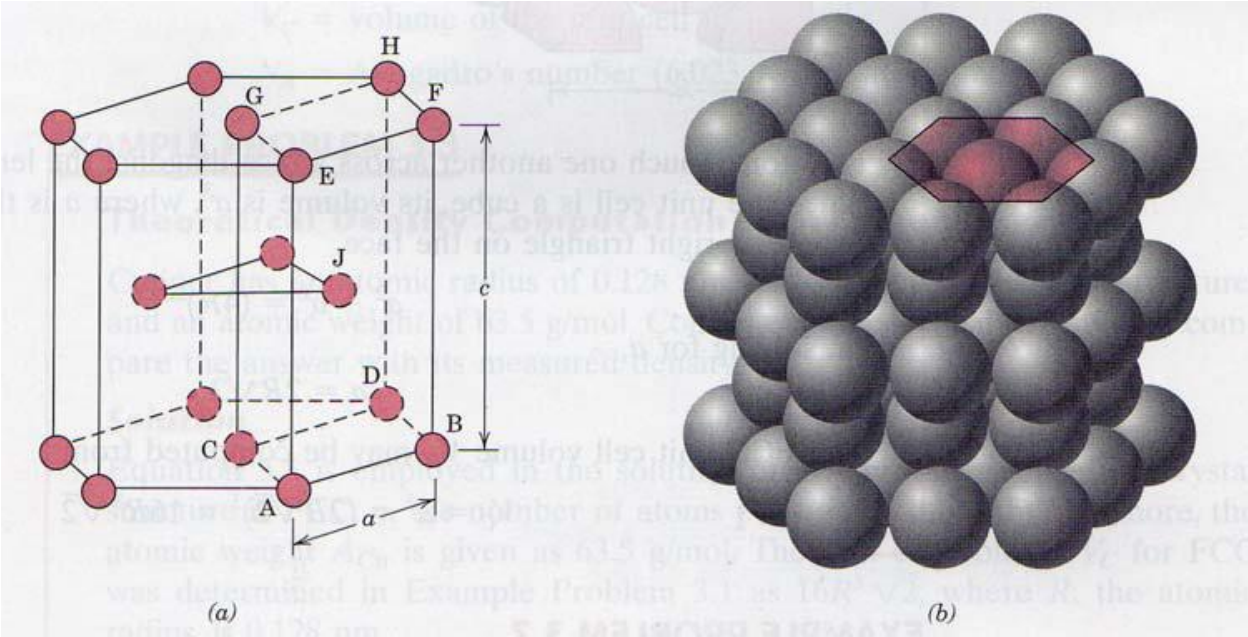
$= (4R/\sqrt{3})^3$

$= 12.32\ R^3$

APF = $8.373R^3 / 12.32\ R^3$

= 0.68

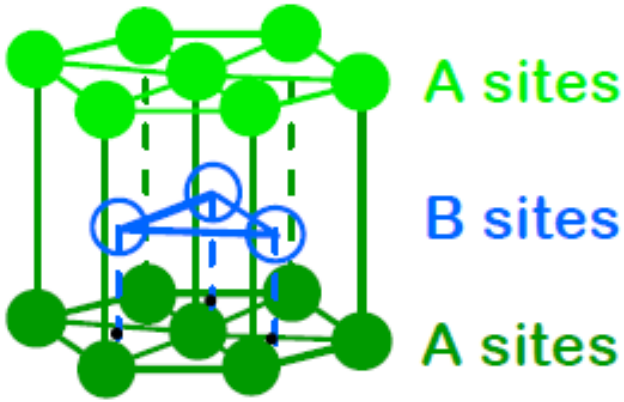
HEXAGONAL CLOSE-PACKED STRUCTURE (HCP)



For HCP crystal structure, (a) a reduced-sphere unit cell: *a* and *c* represent the
short and long edge lengths, respectively), and (b) an aggregate of many atom.

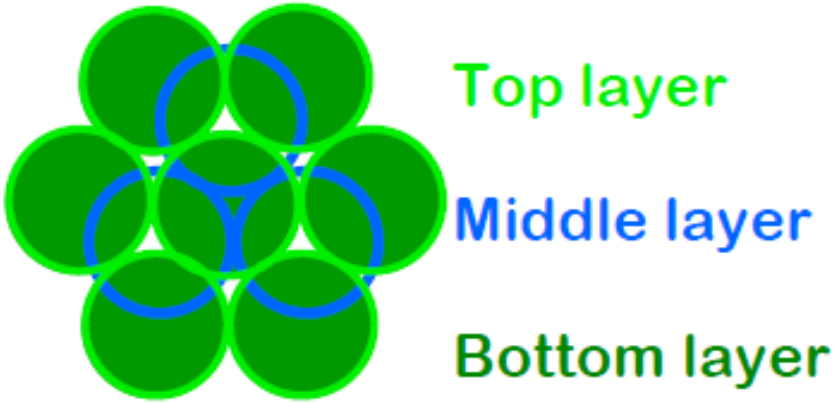
- HCP crystals have the most densely packed configurations, followed by fcc and bcc
- Arrangements can be modified by adding atoms of other metals known as **alloying**.

- 3D Projection



Adapted from Fig. 3.3, *Callister 6e.*

- 2D Projection



Number of atoms in a unit of HCP cell:
No. atom/unit = 6
12 atoms at each corner/6 unit cell = 2
2 atoms at top and bottom of the hexagonal/2 = 1
3 atoms inside the hexagonal = 3

APF = 0.74

THEORETICAL DENSITY, ρ

atoms/unit cell

Atomic weight (g/mol)

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

Volume/unit cell (cm^3/unit cell)

Avogadro's number (6.023×10^{23} atoms/mol)

Characteristics of Selected Elements at 20°C

Element	Symbol	At. Weight (amu)	Density (g/cm^3)	Crystal Structure	Atomic radius (nm)
Aluminum	Al	26.98	2.71	FCC	0.143
Argon	Ar	39.95	------	------	------
Barium	Ba	137.33	3.5	BCC	0.217
Beryllium	Be	9.012	1.85	HCP	0.114
Boron	B	10.81	2.34	Rhomb	------
Bromine	Br	79.90	------	------	------
Cadmium	Cd	112.41	8.65	HCP	0.149
Calcium	Ca	40.08	1.55	FCC	0.197
Carbon	C	12.011	2.25	Hex	0.071
Cesium	Cs	132.91	1.87	BCC	0.265
Chlorine	Cl	35.45	------	------	------
Chromium	Cr	52.00	7.19	BCC	0.125
Cobalt	Co	58.93	8.9	HCP	0.125
Copper	Cu	63.55	8.94	FCC	0.128
Flourine	F	19.00	------	------	------
Gallium	Ga	69.72	5.90	Ortho.	0.122
Germanium	Ge	72.59	5.32	Dia. cubic	0.122
Gold	Au	196.97	19.32	FCC	0.144
Helium	He	4.003	------	------	------
Hydrogen	H	1.008	------	------	------

Example 4: Copper

Data from Table inside front cover of Callister (see next slide):

- crystal structure = FCC: 4 atoms/unit cell
- atomic weight = 63.55 g/mol (1 amu = 1 g/mol)
- atomic radius R = 0.128 nm (1 nm = 10^{-7} cm)
- Avogadro's number = 6.022 x 10^{23} atoms/mol)

$V_C = a^3$; For FCC, $a = 4R/\sqrt{2}$; $V_C = 4.75 \times 10^{-23} cm^3$

$$\rho = \frac{nA}{V_c N_A}$$

Result: theoretical $\rho_{Cu} = 8.89\ g/cm^3$

EXAMPLE PROBLEM 3.3

Theoretical Density Computation for Copper

Copper has an atomic radius of 0.128 nm, an FCC crystal structure, and an atomic weight of 63.5 g/mol. Compute its theoretical density and compare the answer with its measured density.

Solution

Equation 3.5 is employed in the solution of this problem. Since the crystal structure is FCC, n, the number of atoms per unit cell, is 4. Furthermore, the atomic weight A_{Cu} is given as 63.5 g/mol. The unit cell volume V_C for FCC was determined in Example Problem 3.1 as $16R^3\sqrt{2}$, where R, the atomic radius, is 0.128 nm.

Substitution for the various parameters into Equation 3.5 yields

$$\rho = \frac{nA_{Cu}}{V_C N_A} = \frac{nA_{Cu}}{(16R^3\sqrt{2})N_A}$$

$$= \frac{(4 \text{ atoms/unit cell})(63.5 \text{ g/mol})}{[16\sqrt{2}(1.28 \times 10^{-8} \text{ cm})^3/\text{unit cell}](6.023 \times 10^{23} \text{ atoms/mol})}$$

$$= 8.89 \text{ g/cm}^3$$

The literature value for the density of copper is 8.94 g/cm^3, which is in very close agreement with the foregoing result.

DENSITIES OF MATERIAL CLASSES

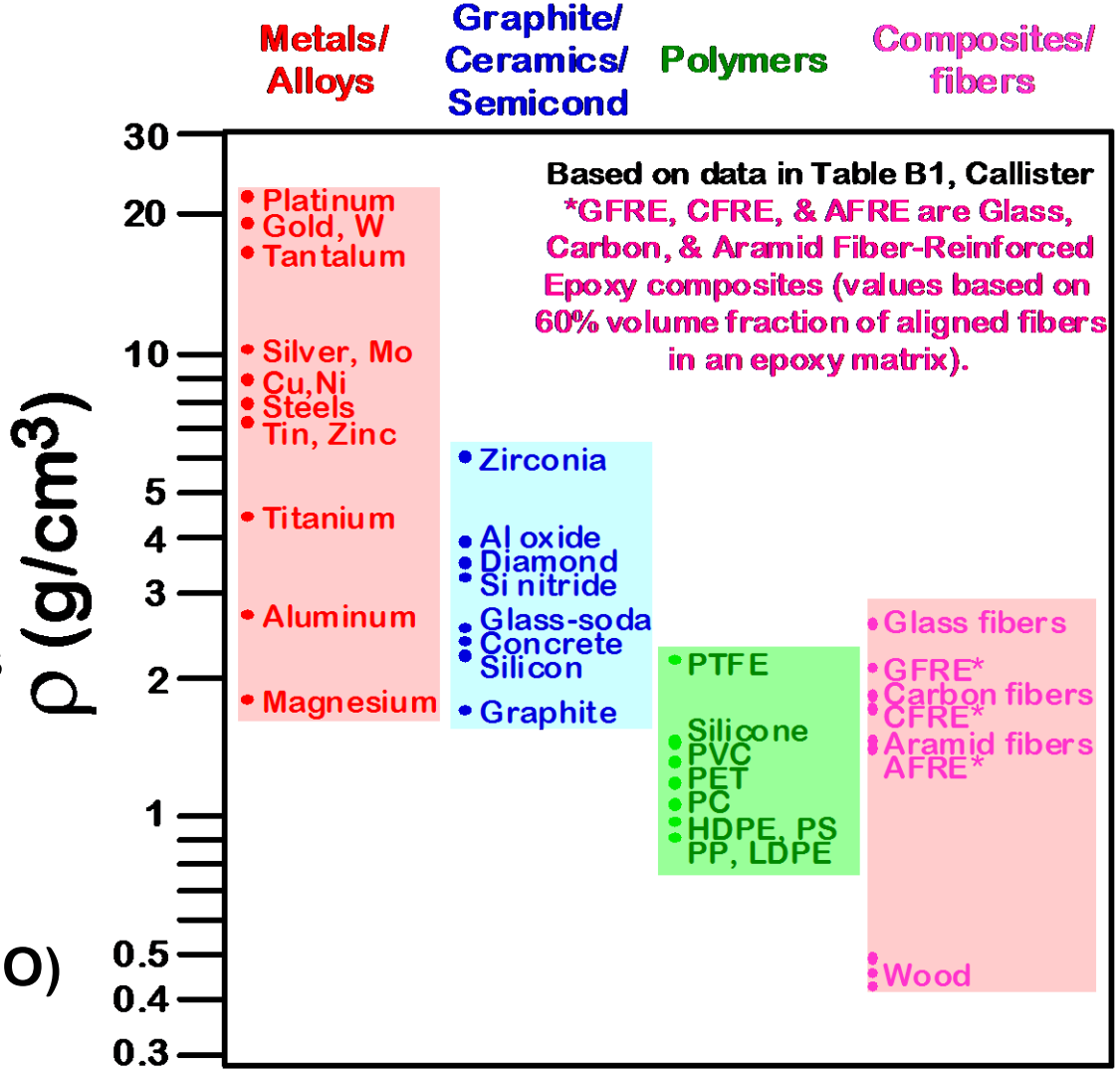
Why?

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

Ceramics have...
- less dense packing (covalent bonding)
- often lighter elements

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

Composites have...
- intermediate values



Data from Table B1, *Callister 6e.*

Single crystal and polycrystalline materials

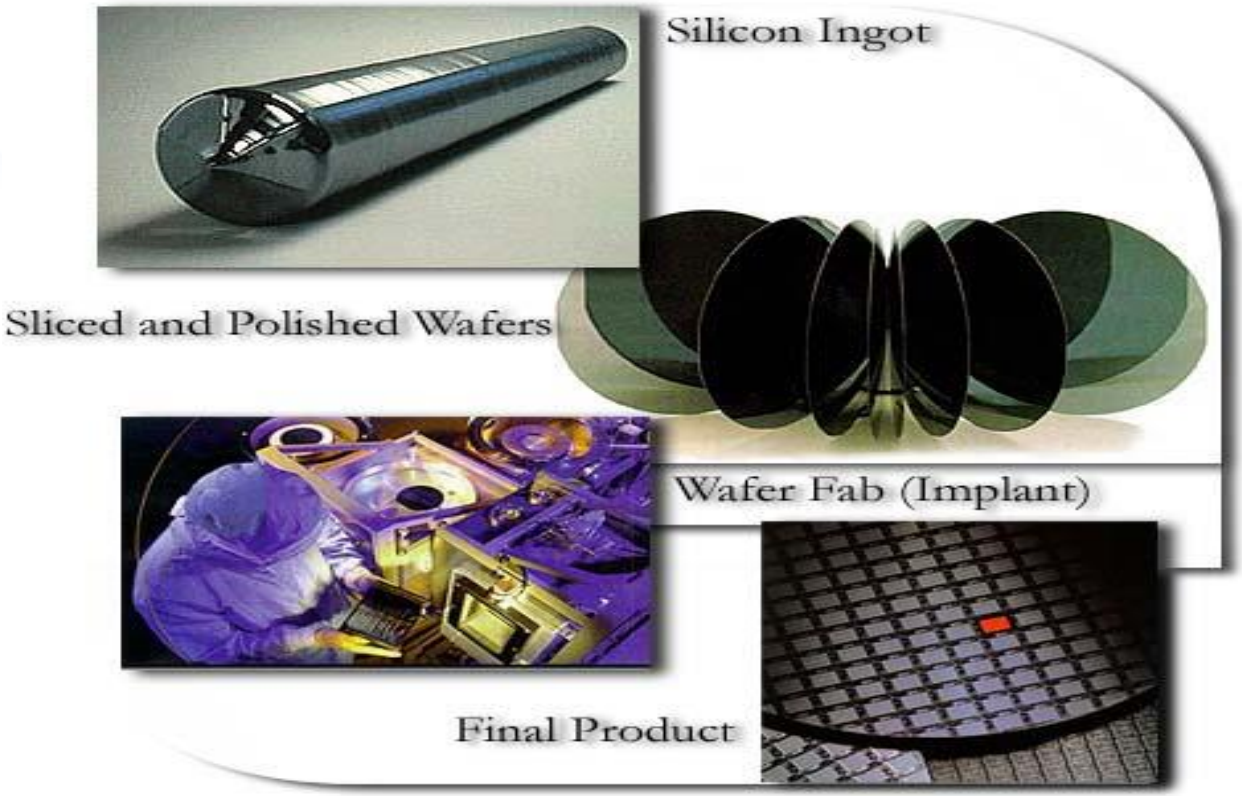
Single crystal ➔ Periodic and repeated arrangement of atoms is perfect or extends throughout the entirety of specimen without interruption.

Only 1 Crystal – environment must be carefully controlled

All unit cells interlock in the same way & have same orientation, geometry shape having flat surface.

Single crystal

- ***Some*** **engineering applications require single crystals:**



Semiconductor- single crystal are necessary to allow electron flow more 'easily' w/out disturbance of grain boundaries

POLYCRYSTALS

- ***Most*** **engineering materials are polycrystals.**
  Composed of collection of many small crystals or grain

1 mm

Adapted from Fig. K, color inset pages of *Callister 6e*. (Fig. K is courtesy of Paul E. Danielson, Teledyne Wah Chang Albany)

- **Crystal sizes typ. range from 1 nm to 2 cm**
  (i.e., from a few to millions of atomic layers).

POLYMORPHISM AND ALLOTROPHY

POLYMORPHISM: Polymorphism is the ability of a solid material to exist in more than one form or crystal structure.
Example: Silica is known to form many polymorphs, the most important of which are; α-quartz, β-quartz, tridymite, cristobalite, coesite, and stishovite

ALLOTROPHY: Allotropy or allotropism is the property of some chemical elements to exist in two or more different forms.
Example: Carbon, the allotropes of carbon include diamond (where the carbon atoms are bonded together in a tetrahedral lattice arrangement), graphite (where the carbon atoms are bonded together in sheets of a hexagonal lattice).

Note: Polymorphism and Allotropy are same thing. Polymorphism is used for compounds and the allotropy is reserved for elements.

X-Ray Diffraction

How we identified this ‘white powder’?

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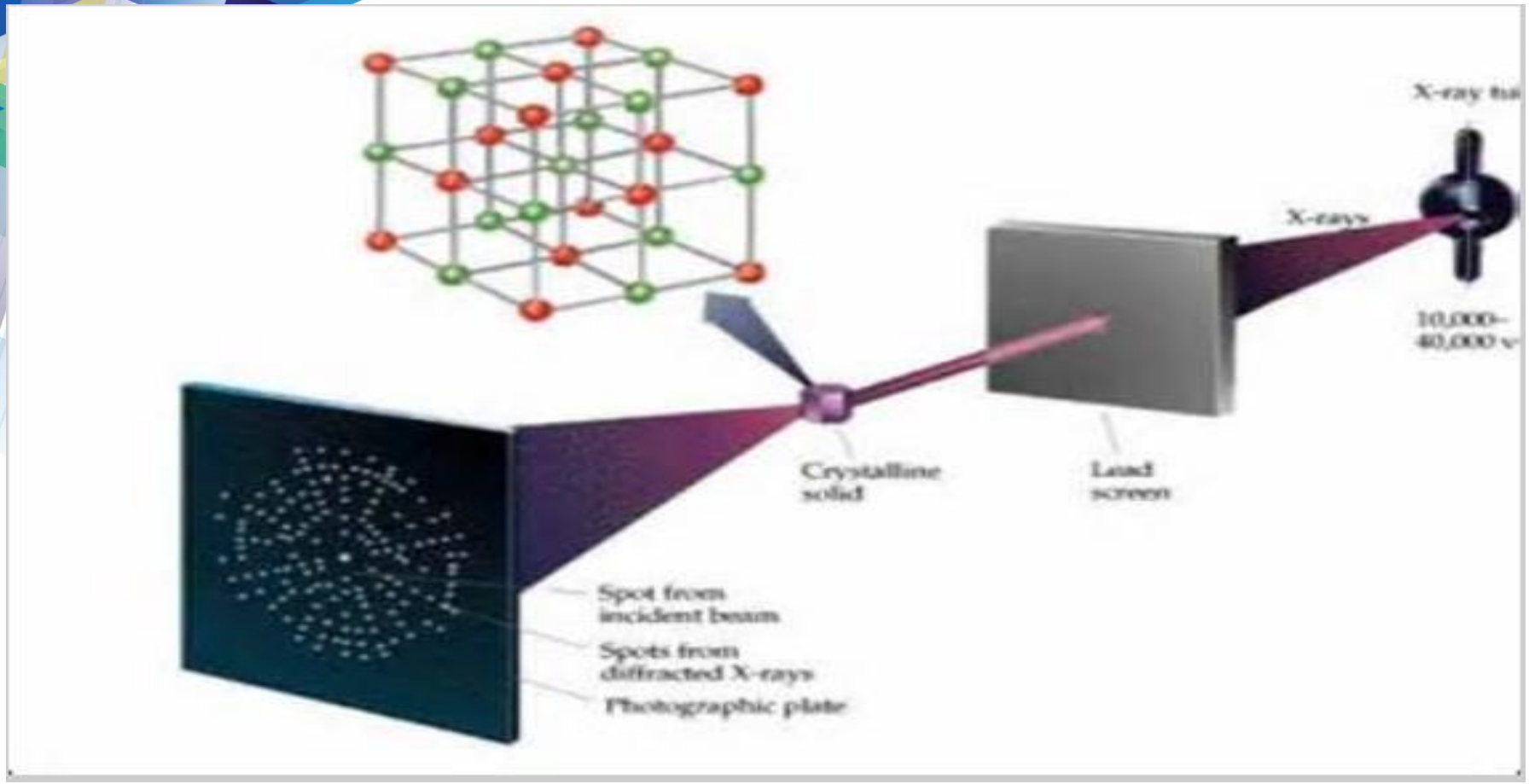

Why X-ray Diffraction (XRD)?

- We can understand atomic and molecular arrangements in solids.
  - Crystal structures & type of materials.
- We can development new materials

4. Imperfection in solids

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Topic Contents

- **Introduction**
  - Solidification
  - Microscopic Examination
- **Point Defect**
  - Vacancies and Self-Interstitials
  - Impurities in Solid
  - Specification of Composition
- **Miscellaneous Imperfections**
  - Dislocations – Linear Defects
  - Interfacial Defects
  - Bulk or Volume Defects

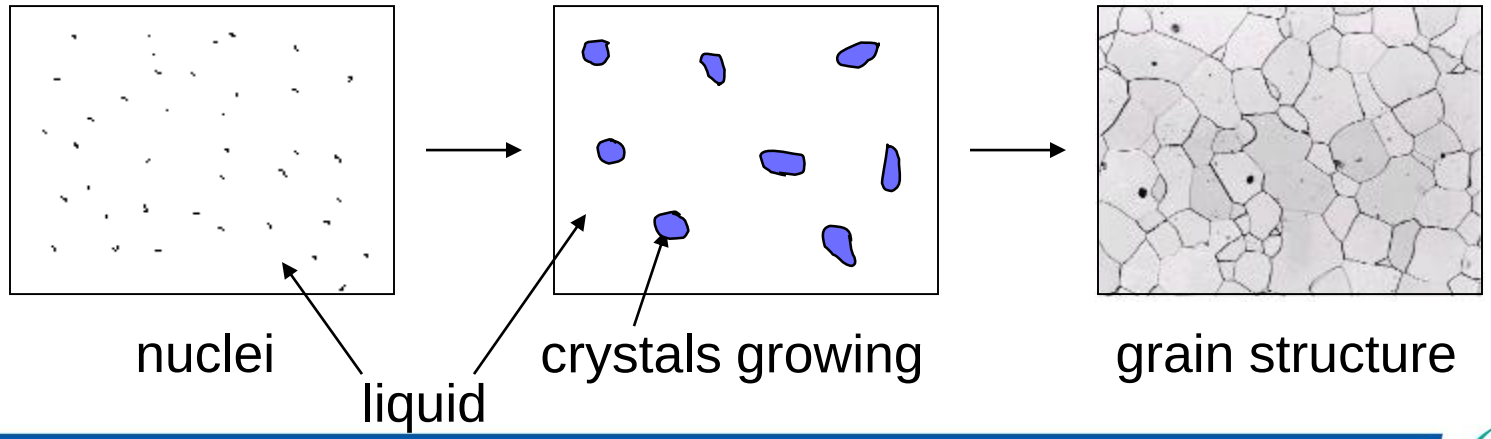
INTRODUCTION

ISSUES TO ADDRESS...

- What are the solidification mechanisms?
- What types of defects arise in solids?
- Can the number and type of defects be varied and controlled?
- How do defects affect material properties?
- Are ALL defects undesirable?

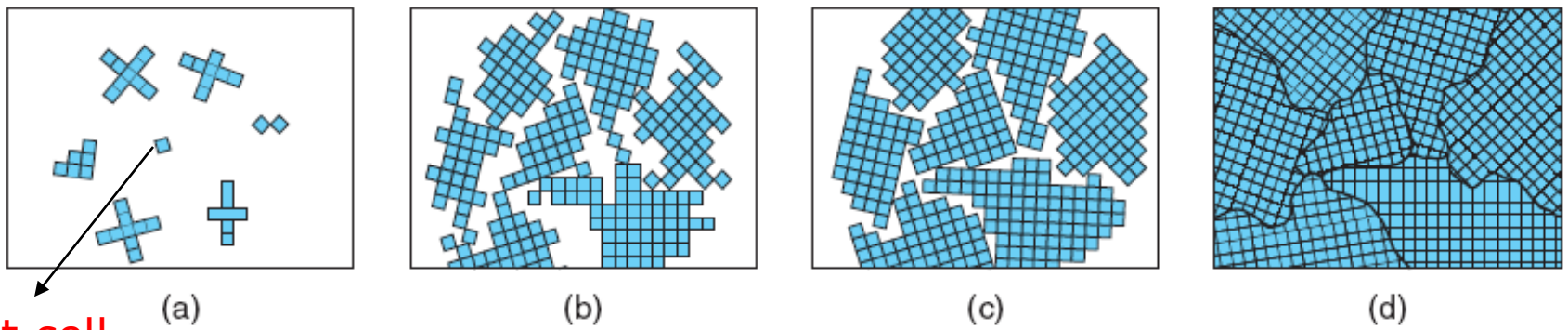
Solidification

- The solidification of metal & alloy - important industrial process
- Most metal are melted & then cast into semifinished or finished shape.
- Solidification- result of casting of molten material
    - Nuclei form
    - Nuclei grow to form crystals – grain structure
- Start with a molten material – all liquid
- Crystals grow until they meet each other



Stages of solidification of polycrystalline material

Cooling Process

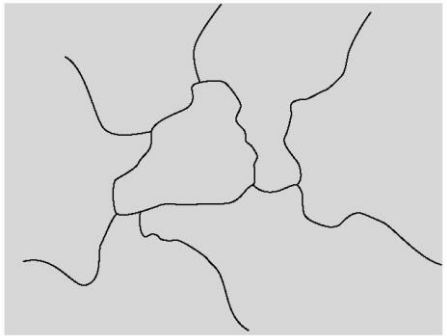


Unit cell

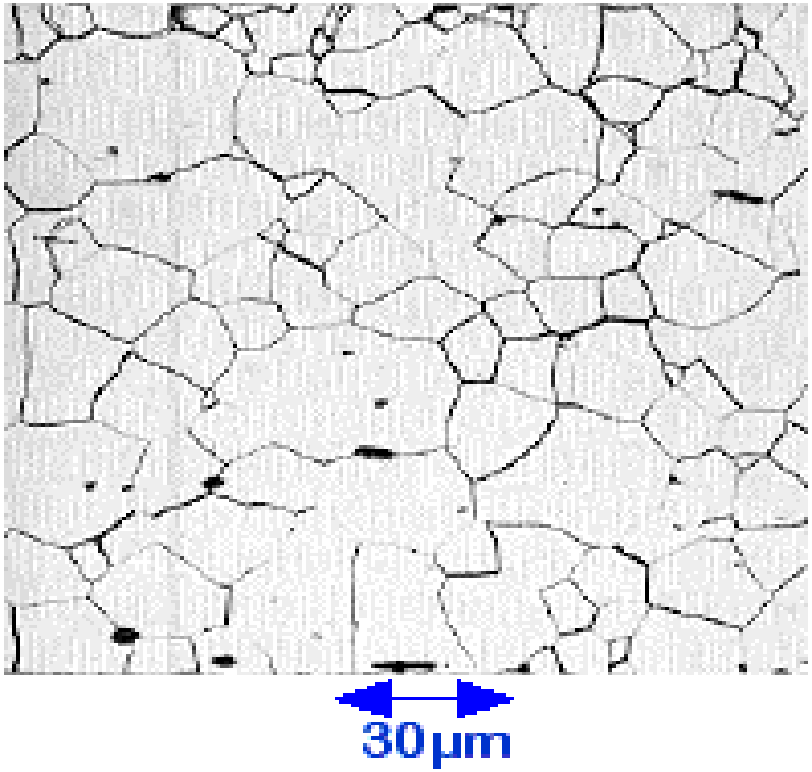
a) Small crystallite nuclei (molten)

b) Growth of the crystallites; the obstruction (block) of some grains that are adjacent to one another have formed

c) Upon completion of solidification, grains (atomic mismatch) having irregular shapes have formed



d) The grain structure as it would appear under the microscope (dark lines are the grain boundary)



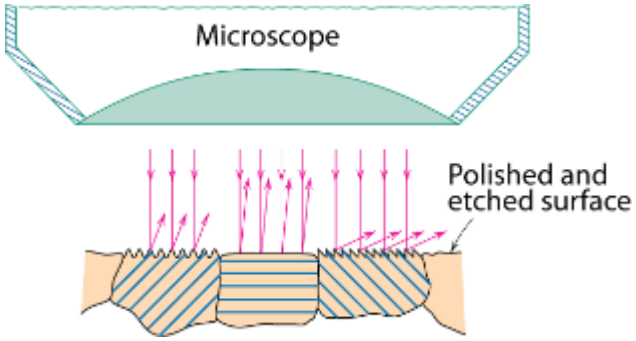
- Solidified metal containing many crystal is said to be polycrystalline.
- Number and size of the grains depends on the *rate* at which **nucleation** takes place
- The crystal in the solidified metal are called grains and the surface between them, grain boundaries.

Microscopic Examination

- Crystallites (grains) and grain boundaries. Vary considerably in size. Can be quite large
  - ex: Large single crystal of quartz or diamond or Si
  - ex: Aluminum light post or garbage can - see the individual grains
- Crystallites (grains) can be quite small (mm or less) – necessary to observe with a microscope.

Optical Microscopy

- Useful up to 2000X magnification.
- Polishing removes surface features (e.g., scratches); surface like mirror
- Etching changes reflectance, depending on crystal orientation.



0.75mm

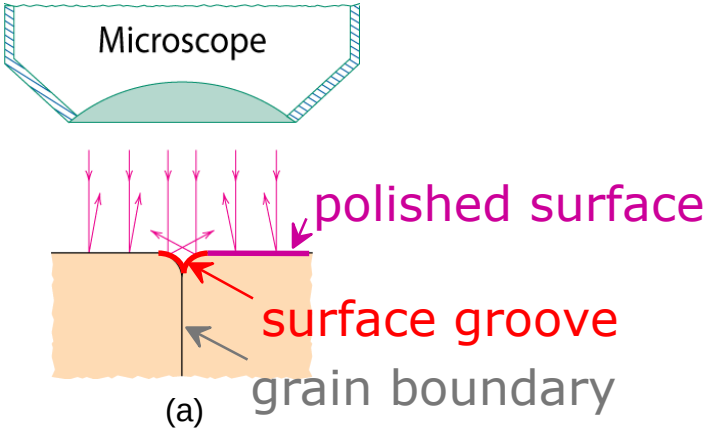
Micrograph of brass (a Cu-Zn alloy)

Adapted from Fig. 4.13(b) and (c), *Callister 7e.* (Fig. 4.13(c) is courtesy of J.E. Burke, General Electric Co.

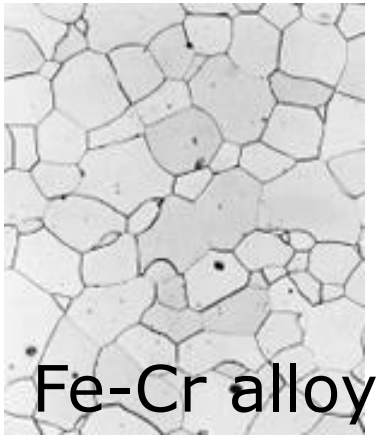
Optical Microscopy

Grain boundaries...

- may be revealed as dark lines,
- change in crystal orientation across boundary.



(a)



(b)

Electron Microscope

- Electron Microscope:

i. The Scanning Electron Microscope (SEM)

ii. Transmission Electron Microscopy (TEM)

i. The Scanning Electron Microscope (SEM)

- The upper limit of optical microscope ~2000x.
- but, some structural elements are too fine/small.
- need higher magnification
- An image of the structure under investigation is formed using beams of electrons instead of light radiation.

- The surface of a specimen to be examined is scanned with an electron beam, and the reflected (or back-scattered) beam of electron is collected, then displayed at the same scanning rate on a cathode ray tube (similar to a CRT TV screen)

ii. Transmission Electron Microscopy (TEM)

- The image seen with a TEM is formed by an electron beam that passes through specimen.
- Details of internal microstructural features are accessible to observation
- Since solid materials are highly absorptive to electron beams, a specimen must be very thin.
- Magnification 1 000 000x are possible.

Imperfections in Solids

- Before this we assume the arrangement of atoms were perfect.
- But, in reality crystals are never perfect.
- Imperfection/defect – affect many of their physical & mechanical properties.

- So, good or not to us?

- Example:
  - Sterling silver (92.5% Silver, 7.5% copper (impurities)
  - strong & hard compared to pure silver.

Types of Imperfections

- Vacancy atoms
- Interstitial atoms
- Substitutional atoms

} **Point defects**

- Edge dislocations
- Screw dislocations
- Mixed dislocations

} **Line defects**

- Grain Boundaries

Interfacial / Area defects

1.0: Point Defects

i. Vacancy

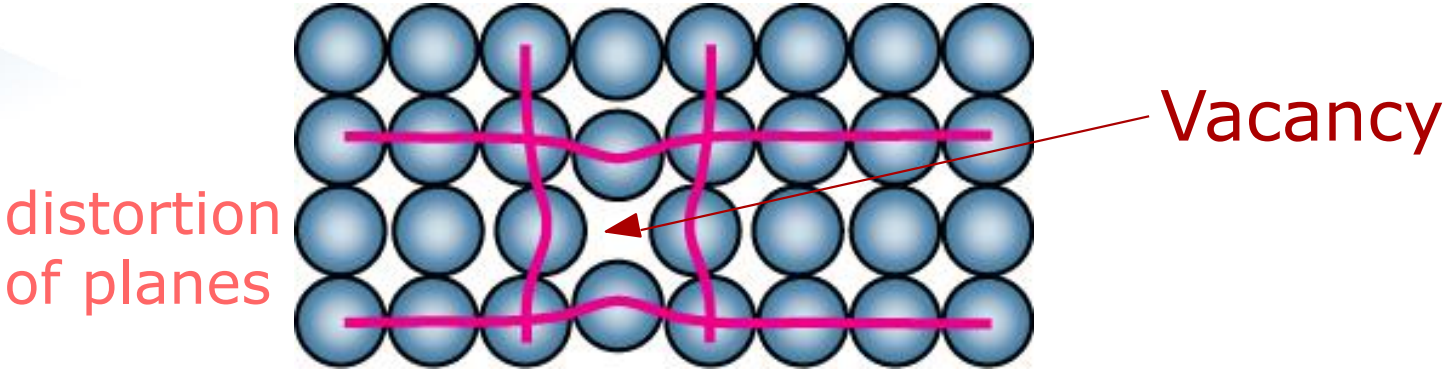
ii. Self-interstitial

iii. Substitutional

i. Vacancies

- Vacancies:

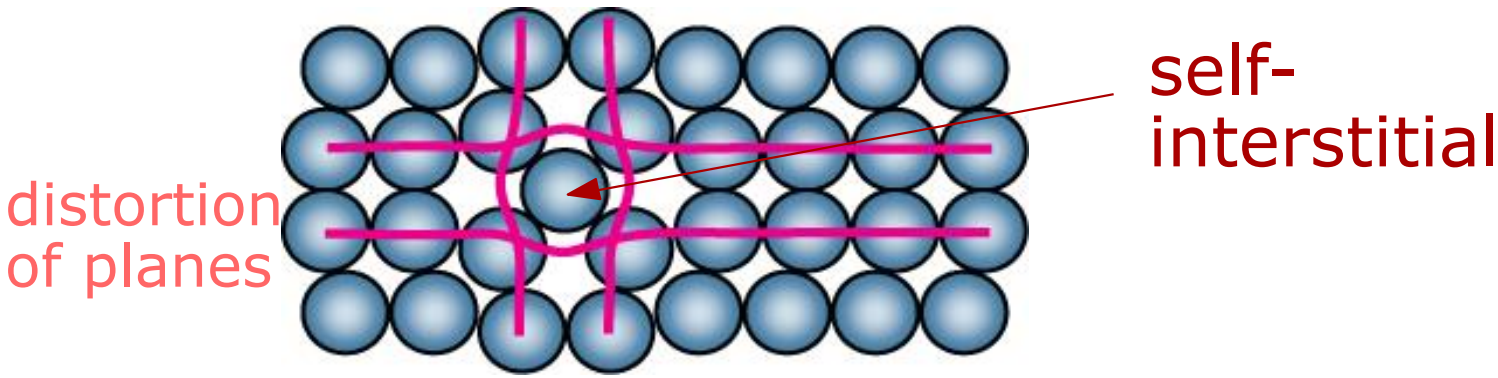
  -vacant atomic sites in a structure.



- The simplest of the point defect – vacancy or vacant lattice site.
- One normally occupied from which an atom is missing
- All crystalline solids contain vacancies.
- Vacancies can moves and exchange site with neighbors

ii. Interstitials

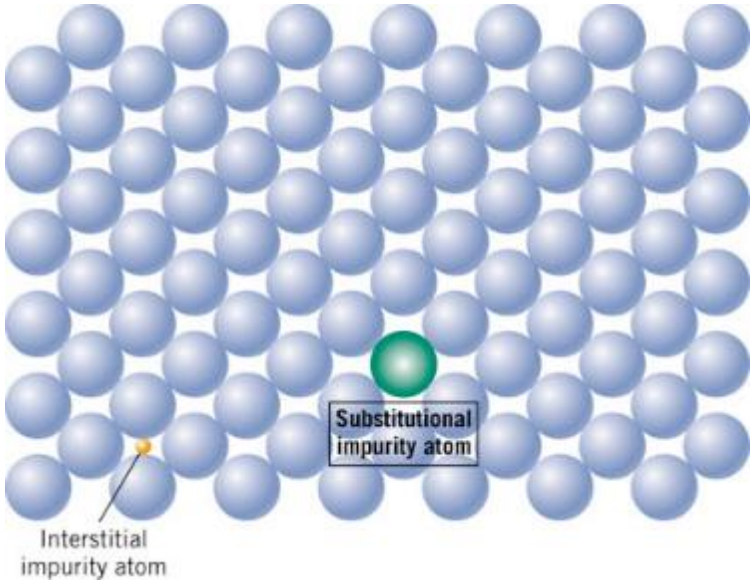
- Interstitials:
  -"extra" atoms positioned between atomic sites.



- An atom from crystal that is crowded into interstitial site.
- A small void space that under ordinary circumstances is not occupied. Impurities atoms fill the voids or interstices among the host atoms.
- In metal – self-interstitial introduces relatively large distortions in the surrounding lattice.
- For metallic materials with high atomic packing factors – interstitial relatively small.
- Example: carbon in FCC Iron – atomic radius difference 42% but carbon can dissolved interstitially in iron

iii. Substitutional

- Solute/impurity atom replace or substitute for the host atoms



Factors: (Hume-Rothery Rules)

i. *Atomic size factor* – impurity atom may be accommodated of solid solution only when the difference in atomic radii between the two types less ± 15%.

ii. *Crystal structure* – for both atom types must be the same.

iii. *Electronegativity* - must be the same

iv. *Valences* - must be the same

Example:

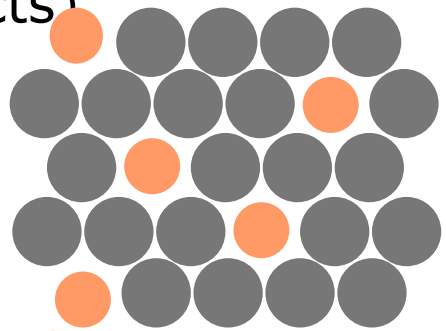
A substitutional solid solution for Cu and Ni

	Cu	*Ni*
Atomic Radius (nm)	0.128	0.125
Crystal Structure	FCC	FCC
Electronegativity	1.9	1.8
Valence	+1/+2	+2

Examples:

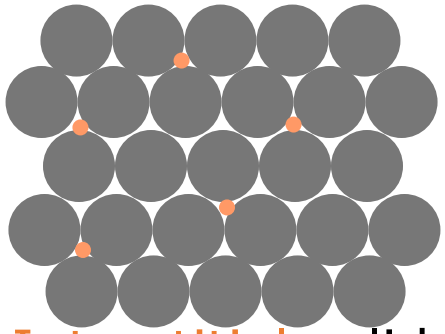
Two outcomes if impurity (B) added to host (A):

- Solid solution of B in A (i.e., random dist. of point defects)



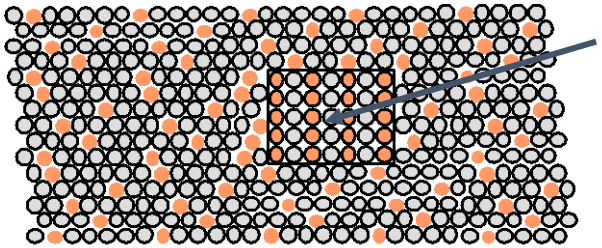
Substitutional solid soln.
(e.g., Cu in Ni)

OR



Interstitial solid soln.
(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

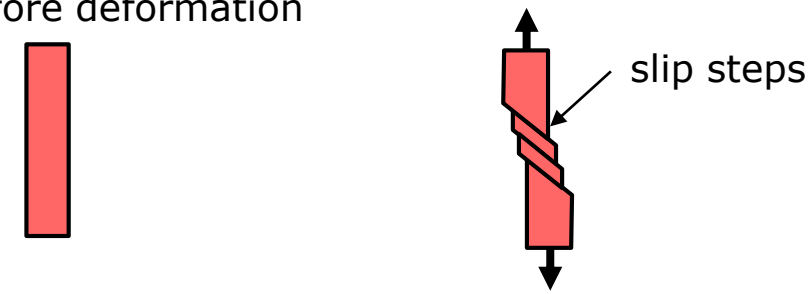
2.0: Linear defects – Dislocations

Linear Defects (Dislocations)

- are one-dimensional defects around which atoms are misaligned
- slip between crystal planes result when dislocations move
- cause Lattice distortation

Schematic of Zinc (HCP):

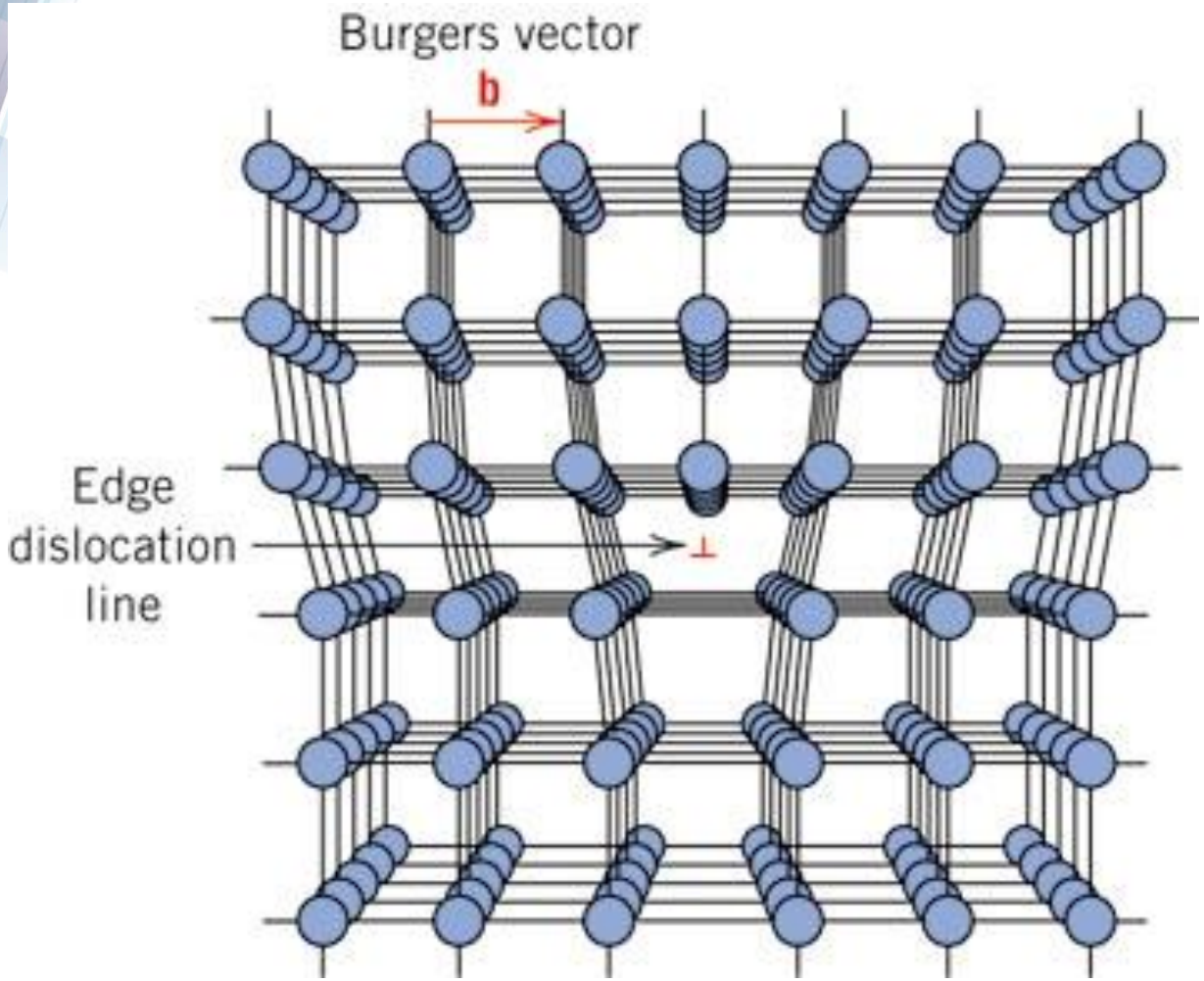
- before deformation
- after tensile elongation



Adapted from Fig. 7.8, *Callister 7e.*

- Edge dislocation:
  - extra half-plane of atoms inserted in a crystal structure
  - **Burger's factor, b** ⊥ to dislocation line. ⊥ (tee :+ve edge dislocation line)
- Screw dislocation:
  - spiral planar ramp resulting from shear deformation
  - **b** || to dislocation line
- Mixed dislocation:
  - Combination of edge and screw dislocation

Edge dislocation

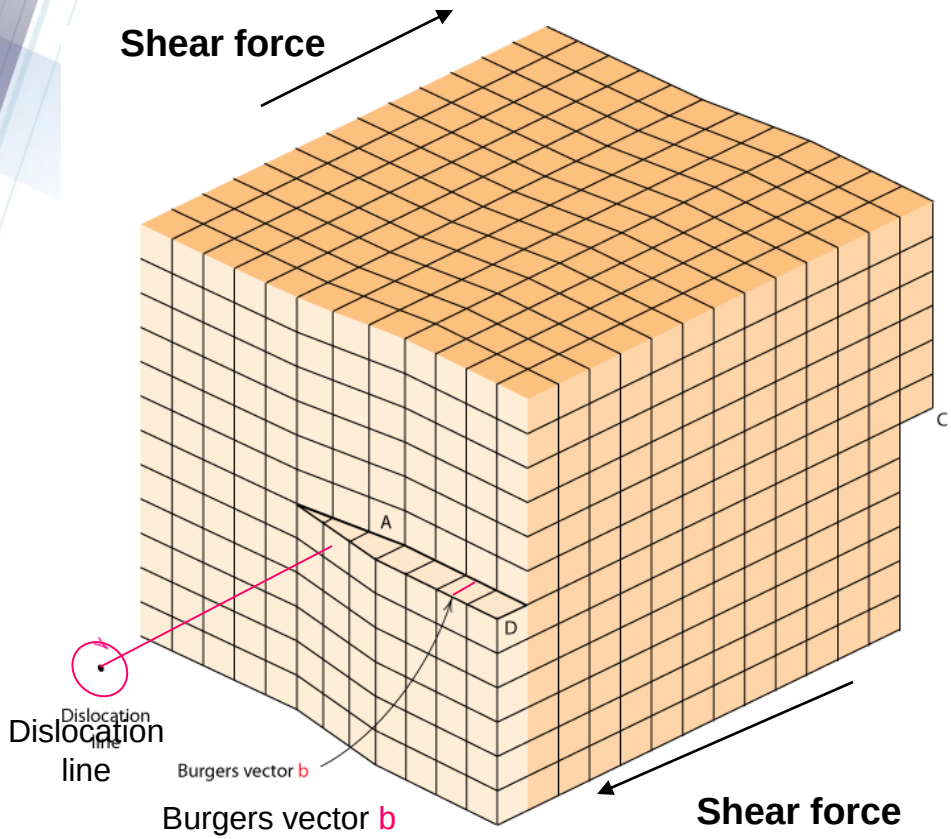


Burger's vector, b: **measure** of lattice distortion

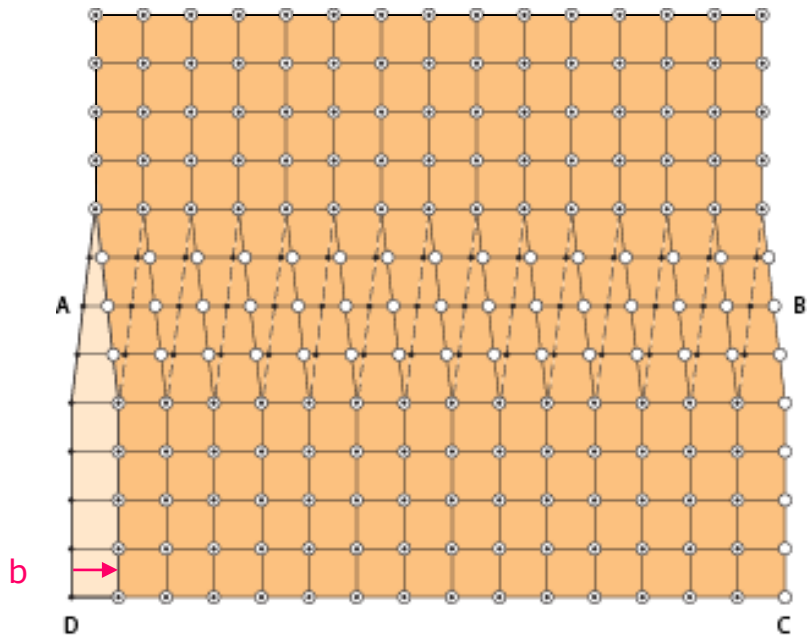
Perpendicular to the edge dislocation line

Screw dislocation

Screw Dislocation

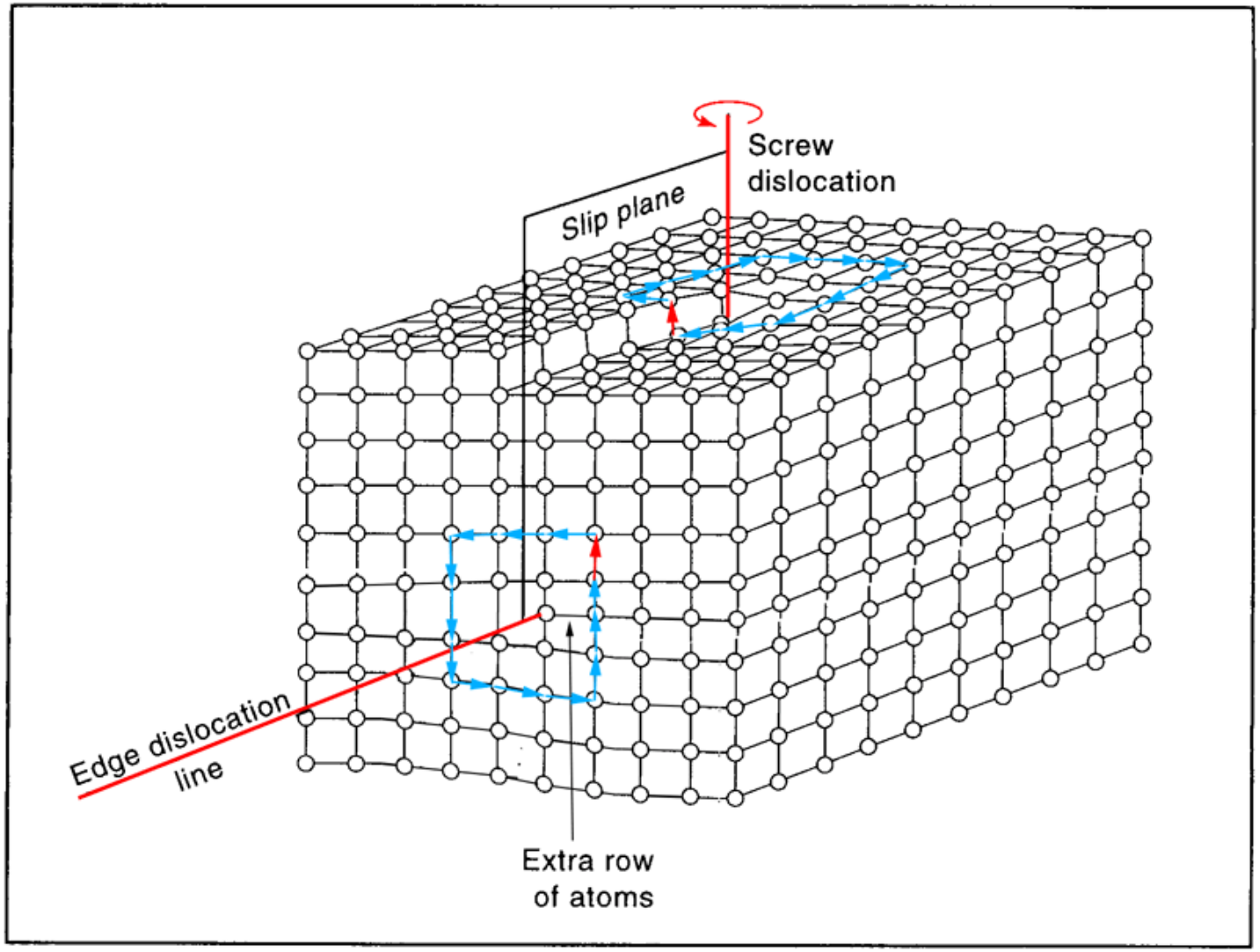


(a)

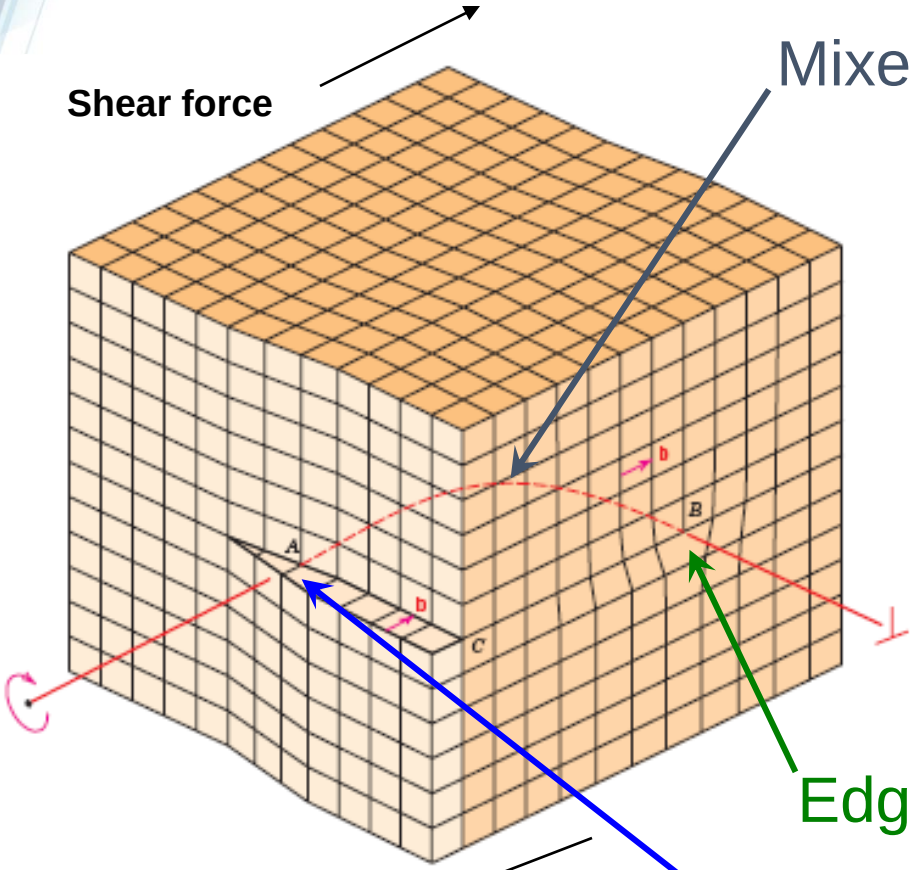


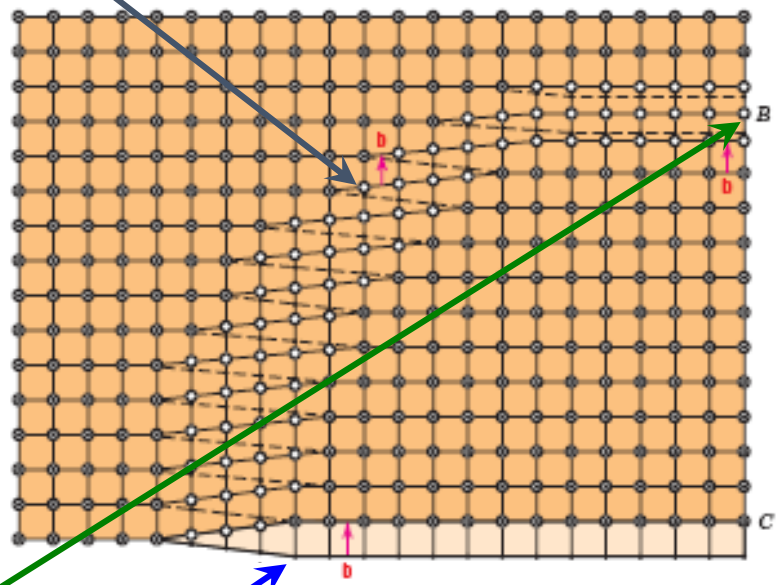
(b)

Shifted one atomic distance (A-B)


Screw
dislocation
Slip plane
Edge dislocation
line
Extra row
of atoms

Edge, Screw, and Mixed Dislocations





Screw dislocation at front surface gradually change to edge dislocation at side of crystal

3.0: Interfacial / Area Defects:

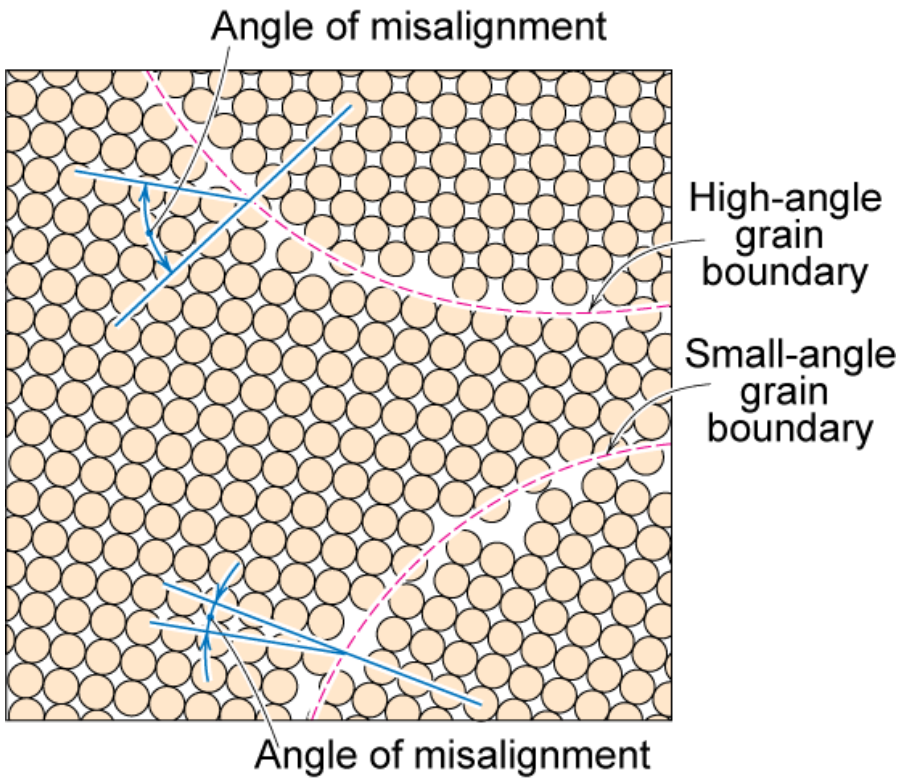
- Grain boundary defect is a boundary that separate two small grains or crystals.

- Examples:
  - External surfaces, grain boundaries, twin boundaries, stacking faults and phase boundaries.

3.0: Interfacial / Area Defects:

- regions between crystals
- transition from lattice of one region to that of the other
- slightly disordered
- Orientation mismatch (angle of misalignment)
- Small angle GB – less surface energy, formed by edge & screw dislocation.

Microstructure in atomic perspective



Adapted from Fig. 4.7, *Callister 7e.*

4.0: Bulk or Volume Defects

- These include pores, cracks foreign inclusion and other phases
- They are normally introduced during processing and fabrication steps.

Summary

- Point, Line, Area and Volume defects exist in solids.
- The number and type of defects can be varied and controlled (e.g., *T* controls vacancy conc.)
- Defects affect material properties (e.g., grain boundaries control crystal slip).
- Defects may be desirable or undesirable (e.g., dislocations may be good or bad, depending on whether plastic deformation is desirable or not.)