

ENGG103 – Materials in Design



UNIVERSITY
OF WOLLONGONG
IN DUBAI



University of Wollongong in Dubai

ENGG103 – Materials in Design

Week 1: Lecture 1 - Atomic Structure, Interatomic Bonding
Crystallinity in Solids, Imperfections

Dr Ciara O'Driscoll

ciaraodriscoll@uowdubai.ac.ae

Consultation:

Tuesday 12:30 – 15:30

Please email first for appointment.



Materials in Design – ENGG103

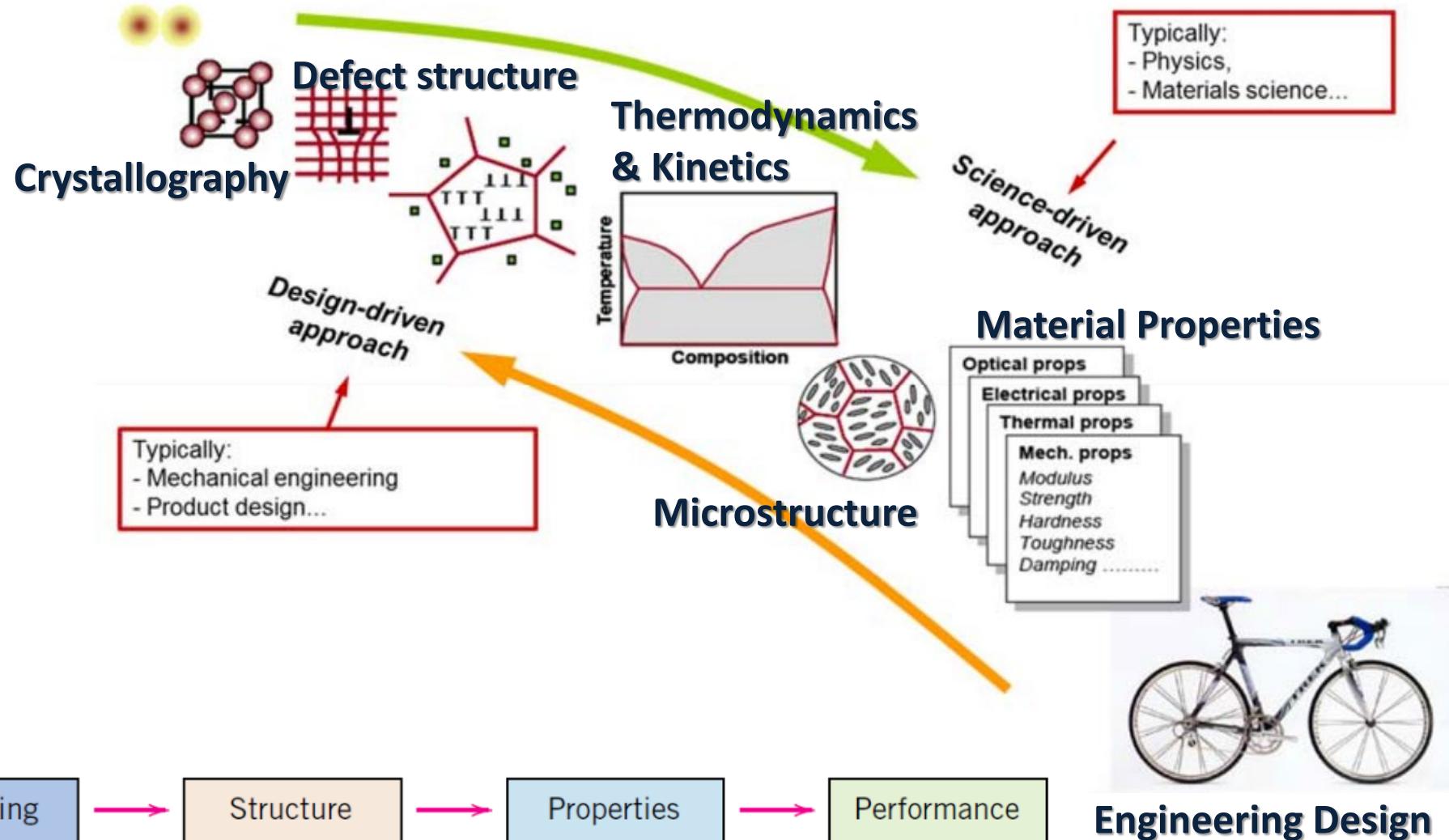


Figure 1.1 The four components of the discipline of materials science and engineering and their interrelationship.



Classification of Materials

On the basis of chemistry and atomic structure, materials are **classified into three general categories:**

1. metals (metallic elements),
2. ceramics (compounds between metallic and nonmetallic elements), and
3. polymers (compounds composed of carbon, hydrogen, and other nonmetallic elements).

In addition, composites are composed of at least two different material types.



- **Mechanical Properties**
 - Modulus
 - Yield and tensile strength
 - Hardness
 - Fracture toughness
- **Thermal Properties**
 - Thermal conductivity
 - Specific heat
 - Thermal Expansion coefficient
 - Melting (solid to liquid)
 - Freezing
 - Vaporisation (Liquid to vapour)
 - Condensation

- **Electrical Properties**

- Resistivity
- Electrical Conduction
- Dielectric behaviour

- **Other Properties**

- Environmental
 - Oxidation
 - Corrosion
 - Wear
- Production
 - Ease of manufacture
 - Joining / Finishing
- Aesthetic
 - Colour/ Texture/ Feel



Types of Materials

- **Metals:**
 - Strong, ductile
 - High thermal & electrical conductivity
 - Opaque, reflective.
- **Polymers/plastics:** Covalent bonding → sharing of e's
 - Soft, ductile, low strength, low density
 - Thermal & electrical insulators
 - Optically translucent or transparent.
- **Ceramics:** ionic bonding (refractory) – compounds of metallic & non-metallic elements (oxides, carbides, nitrides, sulfides)
 - Brittle, glassy
 - Non-conducting (insulators)
- **Composites:** synthetic mixtures of two or more classes of material
 - Matrix phase containing a reinforcing material in the form of particles or fibres

Guest
Lecturer
UOW



The Materials Selection Process

1. Pick Application → Determine required Properties

Properties: mechanical, electrical, thermal,
magnetic, optical

2. Properties → Identify candidate Material(s)

Material: structure, composition.

3. Material → Identify required Processing

Processing: changes *structure* and overall *shape*
ex: casting, sintering, joining, annealing.



SUMMARY

Course Goals:

- Use the right material for the job.
- Understand the relation between properties, structure, and processing.
- Recognize new design opportunities offered by materials selection.



Chapter 2: Atomic Structure & Interatomic Bonding

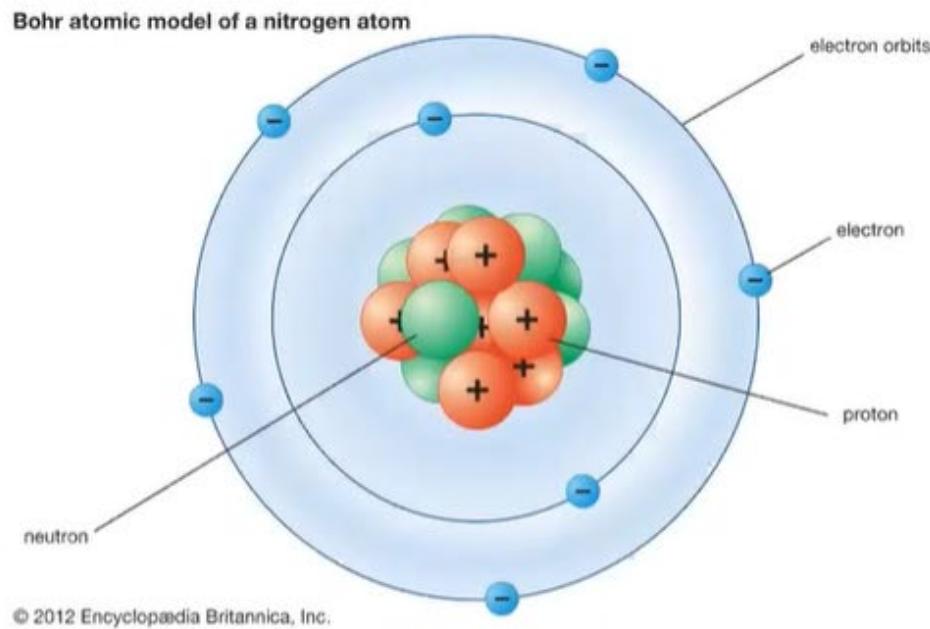
ISSUES TO ADDRESS...

- What promotes bonding?
- What types of bonds are there?
- What properties are inferred from bonding?



ATOMIC STRUCTURE

BOHR ATOMIC MODEL:

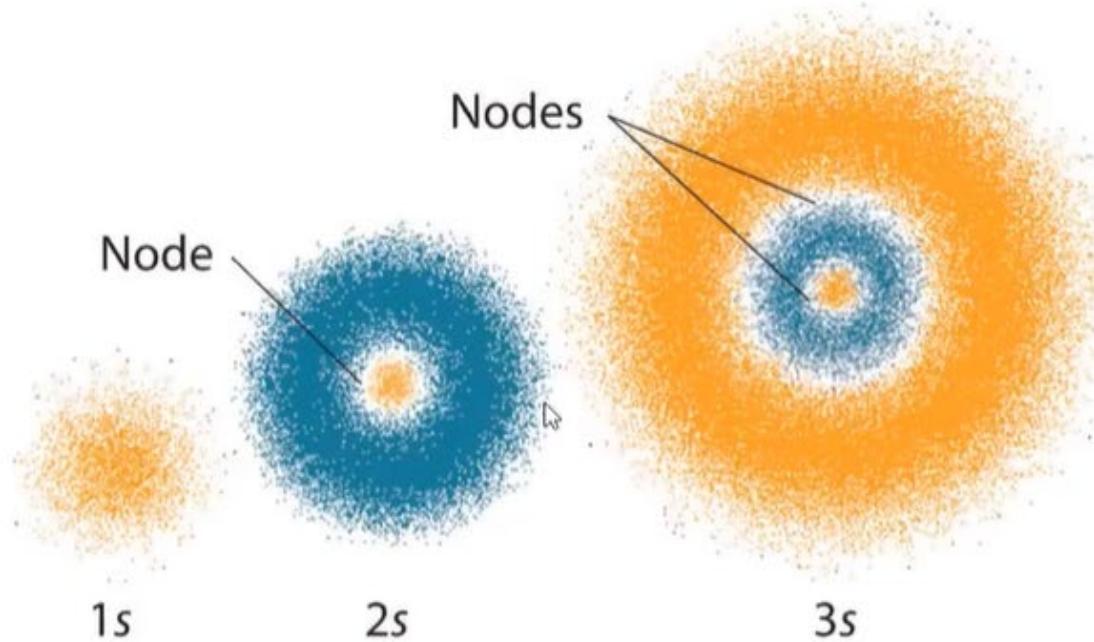


- Each atom has a very small nucleus composed of **protons** and **neutrons**, with **electrons** encircling the nucleus in well-defined orbitals.
- Electrical charge:
 - Electrons: $-1.602 \times 10^{-19} \text{ C}$
 - Protons: $+1.602 \times 10^{-19} \text{ C}$
 - Neutrons: No charge



ATOMIC STRUCTURE

WAVE-MECHANICAL ATOMIC MODEL:



- The location of an electron is treated as the **probability** of the electron being at various locations around the nucleus, and is described by a probability distribution or electron cloud.
- The **electron cloud** is the densest where the probability of finding an electron is the highest.

Understanding the origin of material properties like of Young's Modulus

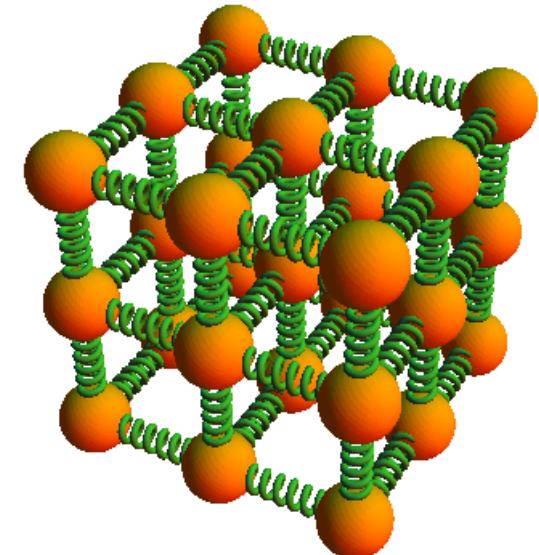
1. Chemical Bond

- Ionic/ covalent/ metallic

2. Atomic Packing

3. BCC/ FCC/ HCP

4. Structure of Crystalline ceramics



Focus on the atomic level

What is a chemical Bond?

A chemical bond is an interaction between two atoms' electrons.

Why do atoms bond?

When atoms don't have a full outer shell of electrons they're more likely to react with other atoms to make their outer shells full.

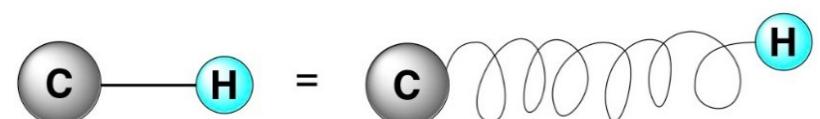
Primary bonds (Strong)

Ceramics & Metals

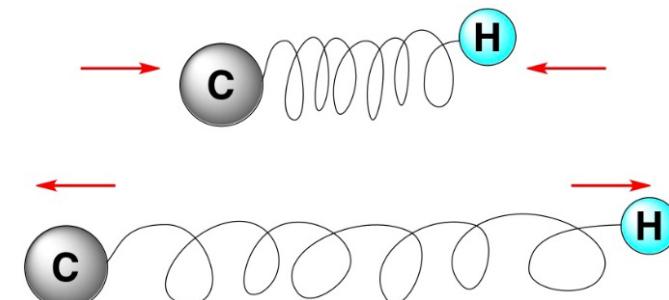
- Ionic
- Covalent
- Metallic

Secondary bonds (Weak)

- Van der Waals bonding
- Hydrogen bonds



Any bond can be thought of as a spring...



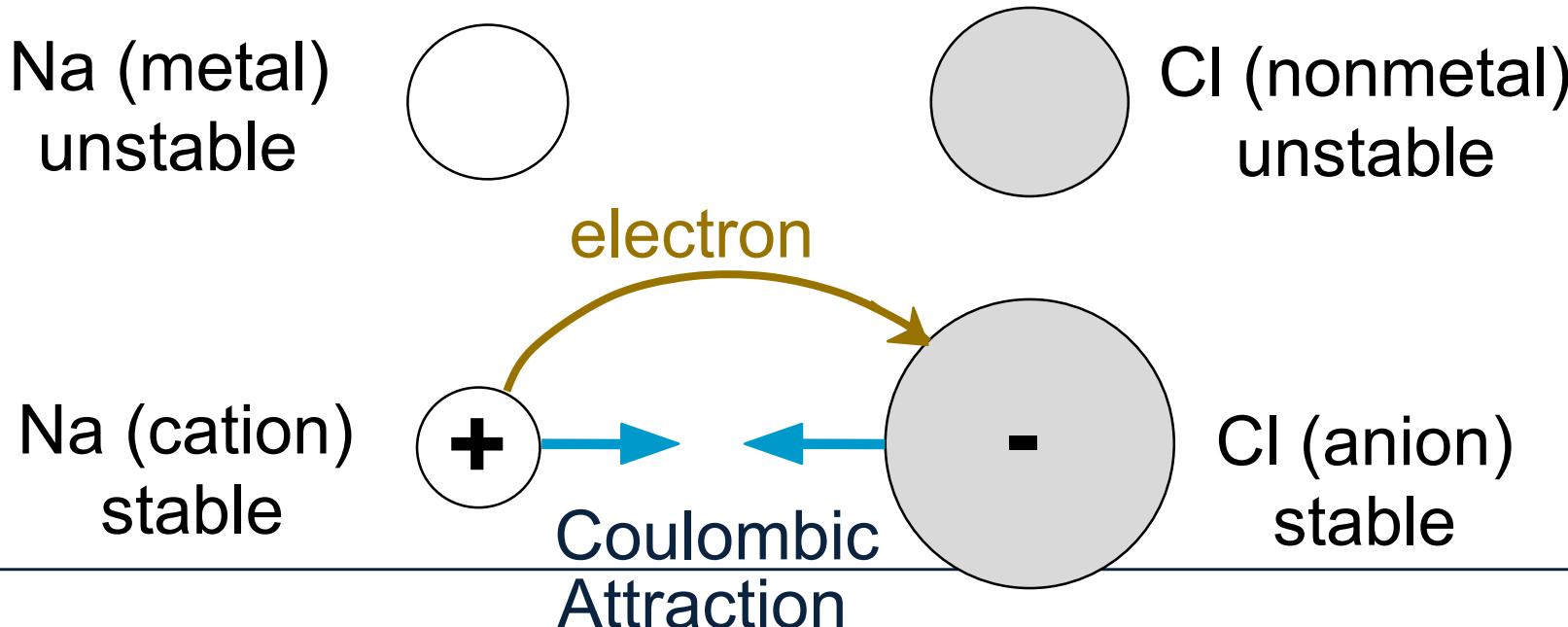
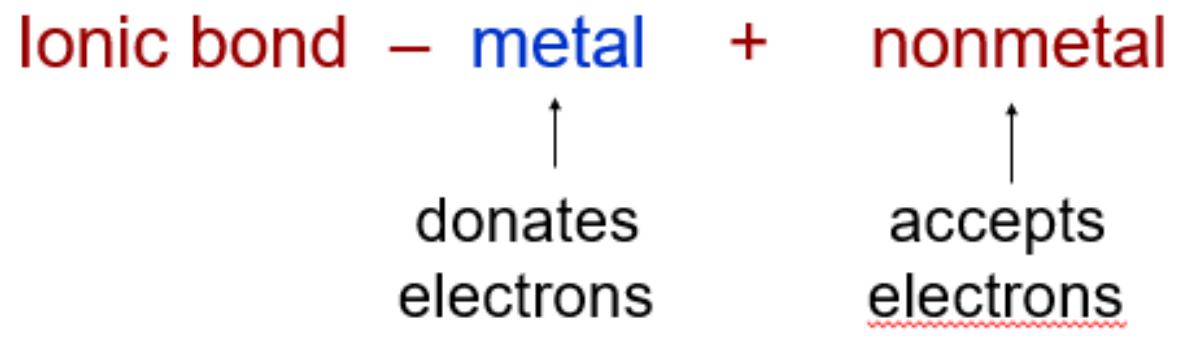
...constantly stretching and contracting.



Ionic Bonding

- Occurs between + and - ions.
- Requires **electron transfer**.
- Large difference in electronegativity required.
- Example: **NaCl**

Na: Sodium
Cl: Chlorine



The Periodic Table

- Columns: Similar Valence Structure

The diagram illustrates the periodic table with annotations for electron gain/loss trends:

- Group 1 (IA):** Hydrogen (H) is highlighted in red. Above it, the text "give up 1e⁻" is written vertically.
- Groups 2 (IIA) and 13 (IIIB):** Lithium (Li) and Magnesium (Mg) are highlighted in red. Between them, the text "give up 2e⁻" is written vertically.
- Groups 13 (IIIB) and 14 (IVB):** Boron (B) and Silicon (Si) are highlighted in blue. Between them, the text "give up 3e⁻" is written vertically.
- Group 17 (VIIA):** Fluorine (F) is highlighted in blue. To its right, the text "accept 1e⁻" is written vertically.
- Group 18 (0):** Helium (He) is highlighted in blue. To its right, the text "inert gases" is written vertically.
- Group 16 (VIA):** Oxygen (O) is highlighted in blue. To its right, the text "accept 2e⁻" is written vertically.
- Group 17 (VIIA):** Chlorine (Cl) is highlighted in blue. To its right, the text "accept 1e⁻" is written vertically.
- Group 18 (0):** Neon (Ne) is highlighted in blue. To its right, the text "inert gases" is written vertically.

Legend:

- Metal: Light blue square
- Nonmetal: Dark blue square
- Intermediate: Light blue diagonal square

Group	Elements
IA	H
IIA	Be
IIIIB	Sc
IVB	Ti
VB	V
VIIB	Cr
VIIIB	Mn
VIII	Fe
IB	Co
IIB	Ni
IIIA	B
IVA	C
VA	N
VIA	O
VIIA	F
0	He
IIIA	Al
IVA	Si
VA	P
VIA	S
VIIA	Cl
0	Ne
IIIA	Ga
IVA	Ge
VA	As
VIA	Se
VIIA	Br
0	Ar
IIIA	Sc
IVA	Zr
VA	Nb
VIA	Mo
VIIA	Tc
0	Ru
IIIA	Rh
IVA	Pd
VA	Ag
VIA	Cd
VIIA	In
0	Sn
IIIA	Sb
IVA	Te
VA	I
VIA	Xe
VIIA	At
0	Rn
Rare earth series	
IIIA	Hf
IVA	Ta
VA	W
VIA	Re
VIIA	Os
0	Ir
IIIA	Pt
IVA	Au
VA	Hg
VIA	Tl
VIIA	Pb
0	Bi
Actinide series	
IIIA	Rf
IVA	Db
VA	Sg
VIA	Bh
VIIA	Hs
0	Mt
IIIA	Ds

Electropositive elements:
Readily give up electrons
to become + ions.

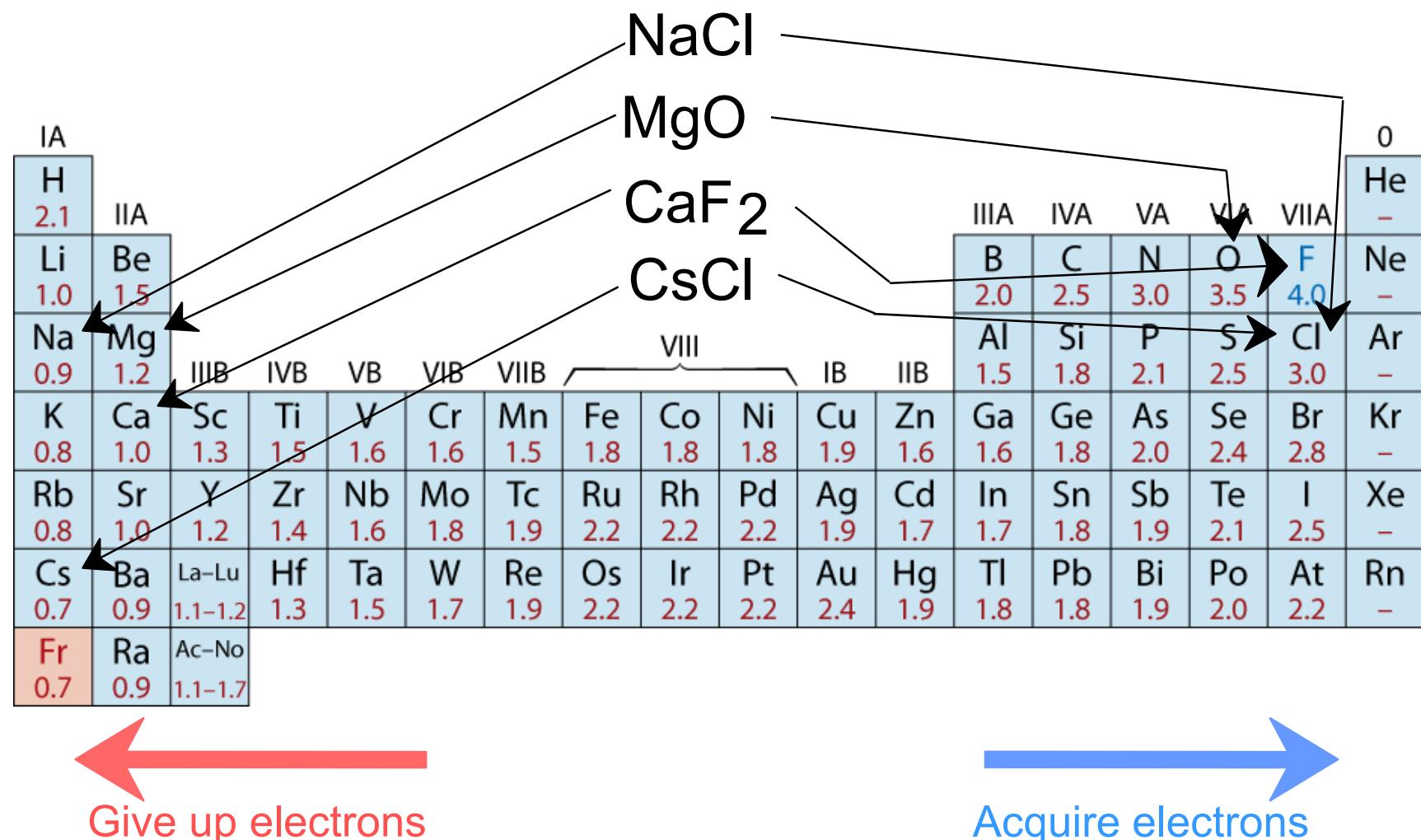
Electronegative elements:
Readily acquire electrons
to become - ions.

Adapted from
Fig. 2.6,
*Callister &
Rethwisch 8e.*



Examples: Ionic Bonding

- Predominant bonding in Ceramics



Adapted from Fig. 2.7, Callister & Rethwisch 8e. (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)



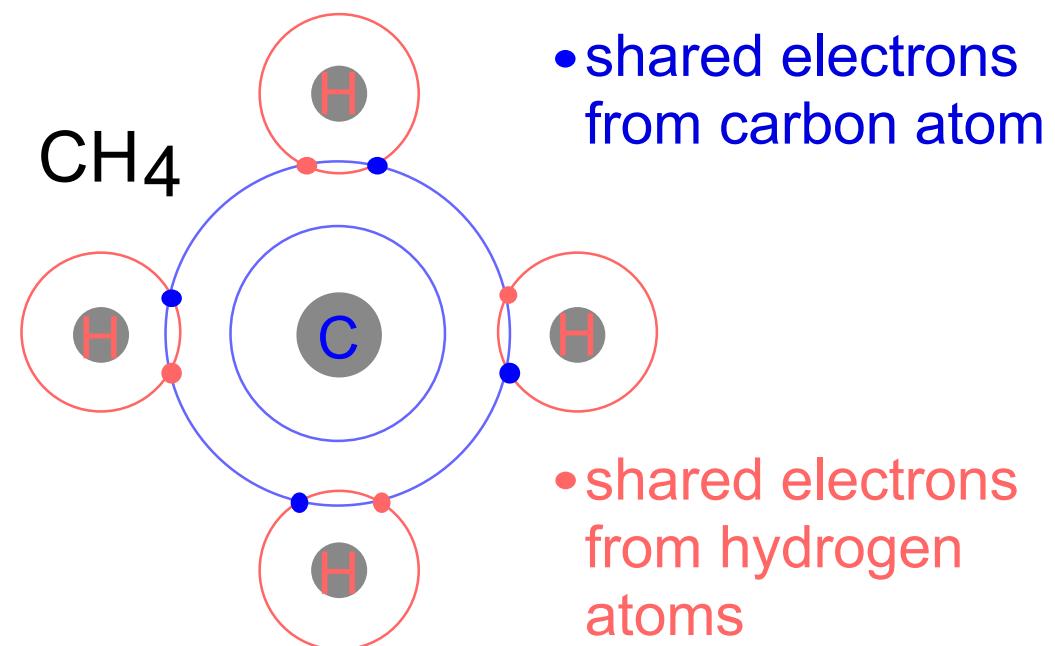
Covalent Bonding

- similar **electronegativity** ∴ share electrons
- bonds determined by valence – s & p orbitals dominate bonding
- Example: CH₄ Methane

C: has 4 valence e⁻, needs 4 more

H: has 1 valence e⁻, needs 1 more

Electronegativities are comparable.



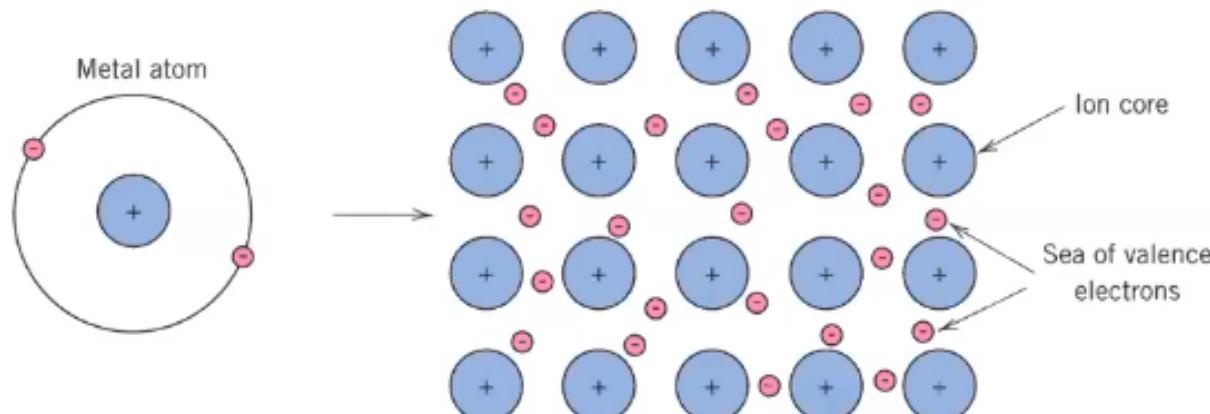
Adapted from Fig. 2.10, Callister & Rethwisch 8e.



ATOMIC BONDING

METALLIC BONDS:

- Metallic bonding occurs in solid metals and alloys, in which the atoms are packed closely enough that their outer valence electrons are attracted to the nuclei of their numerous neighbours.
- The outer valence electrons are therefore not closely attracted to any particular nucleus and are free to drift and spread out among the atoms in the form of a low-density electron charge cloud. The metallic bond is therefore non-directional.
- Solid metals can therefore be visualised as consisting of positive-ion cores (atoms without their outer valence electrons) and valence electrons dispersed in the form of an electron cloud. These valence electrons are weakly bonded to the positive-ion cores and are free to move in the metal crystal structure (often referred to as free electrons).



Chapter 3: The Structure of Crystalline Solids

In order to understand the origin of modulus one needs to know how atoms are packed

ISSUES TO ADDRESS...

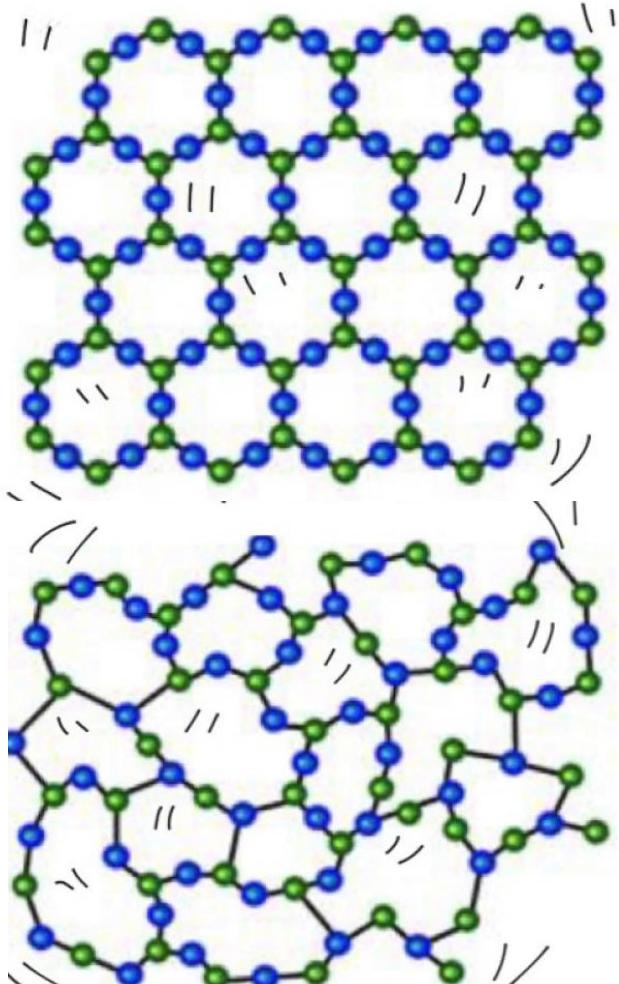
- How do atoms assemble into solid structures?
- How does the density of a material depend on its structure?
- When do material properties vary with the sample (i.e., part) orientation?



Crystalline versus Amorphous

Solid materials can be distinguished according to regularity with which the atoms are arranged in space

- atoms pack in periodic, 3D arrays



Crystalline

Amorphous

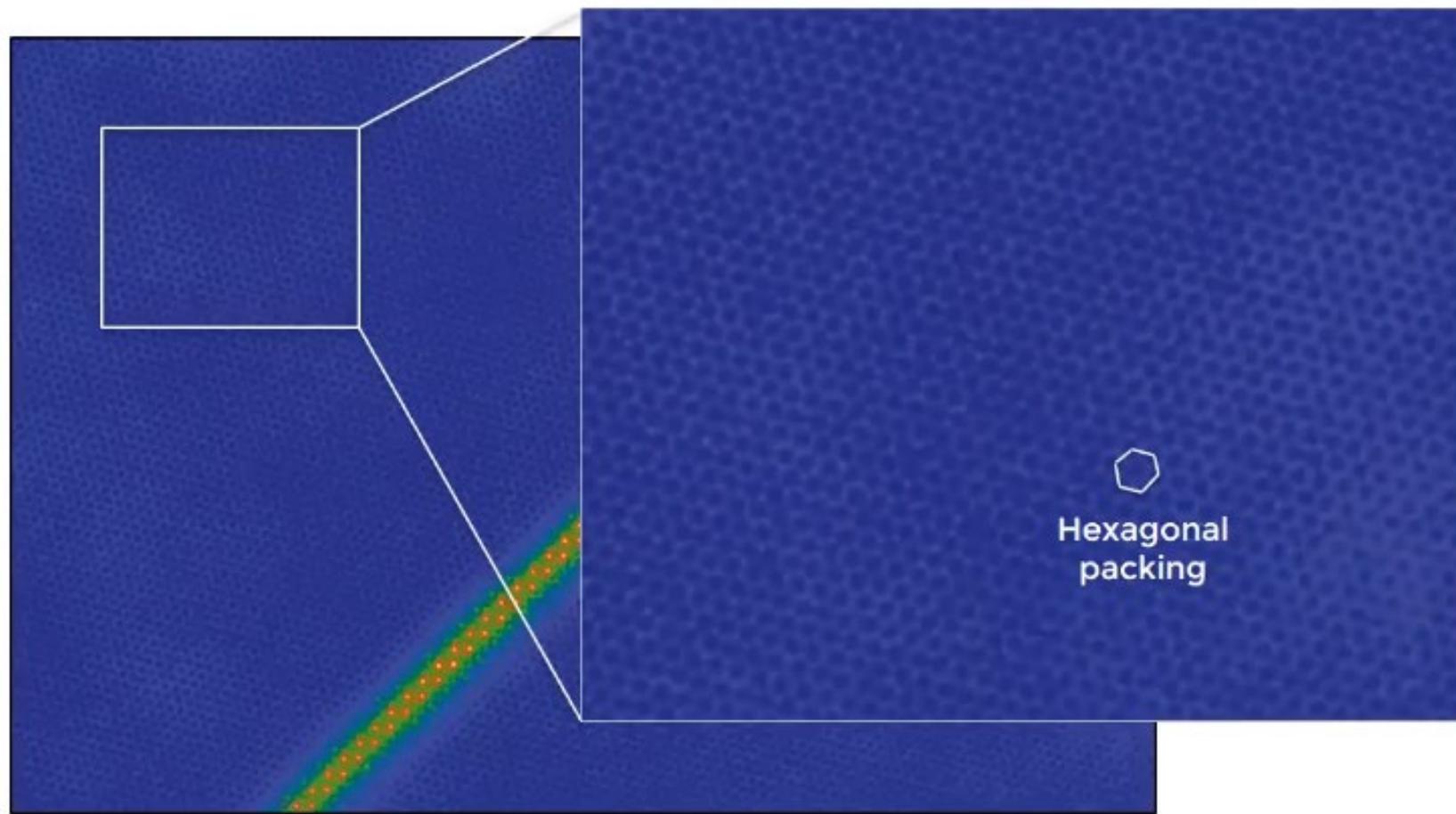
- Uniformly arranged
- Definite characteristics shape
- Long order arrangements
- Sharp melting points
- Rigid, incompressible
 - metals
 - many ceramics
- Diamond

- Randomly arranged
- No definite shape
- short order arrangements
- Melt over a certain temperature
- Glass/Rubber
 - complex structures
 - rapid cooling

- atoms have no periodic packing



METALLIC CRYSTAL STRUCTURES



Aerospace engineers want ultra-strong, light-weight materials to build planes. Magnesium is light, but not very strong. To improve strength, magnesium can be alloyed with 1% calcium and indium (by weight). When added to molten metal, calcium and indium form wafer-thin plates throughout the magnesium. Despite being a mere four atoms wide, these platelets increase the strength of magnesium by a factor of ten.

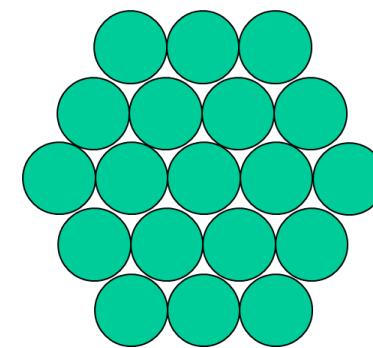


Packing Patterns

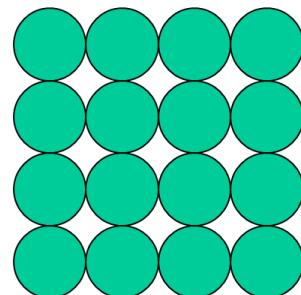
Atom packing

To build up a 3D packing pattern, it is easier conceptually to begin by

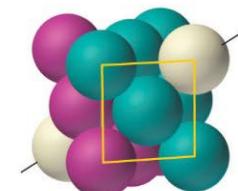
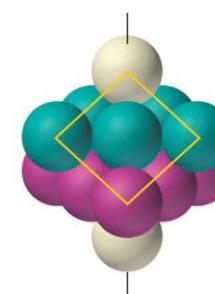
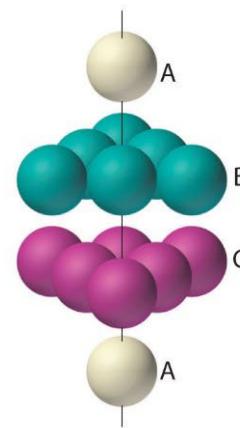
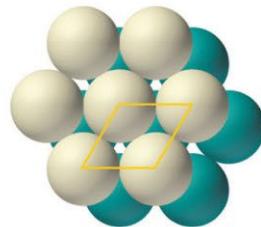
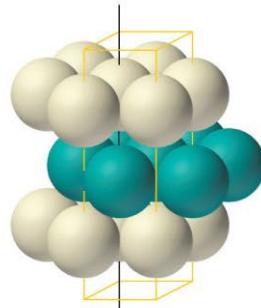
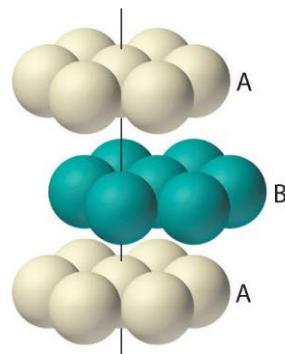
- i. Packing atoms 2D in atomic planes



vs.

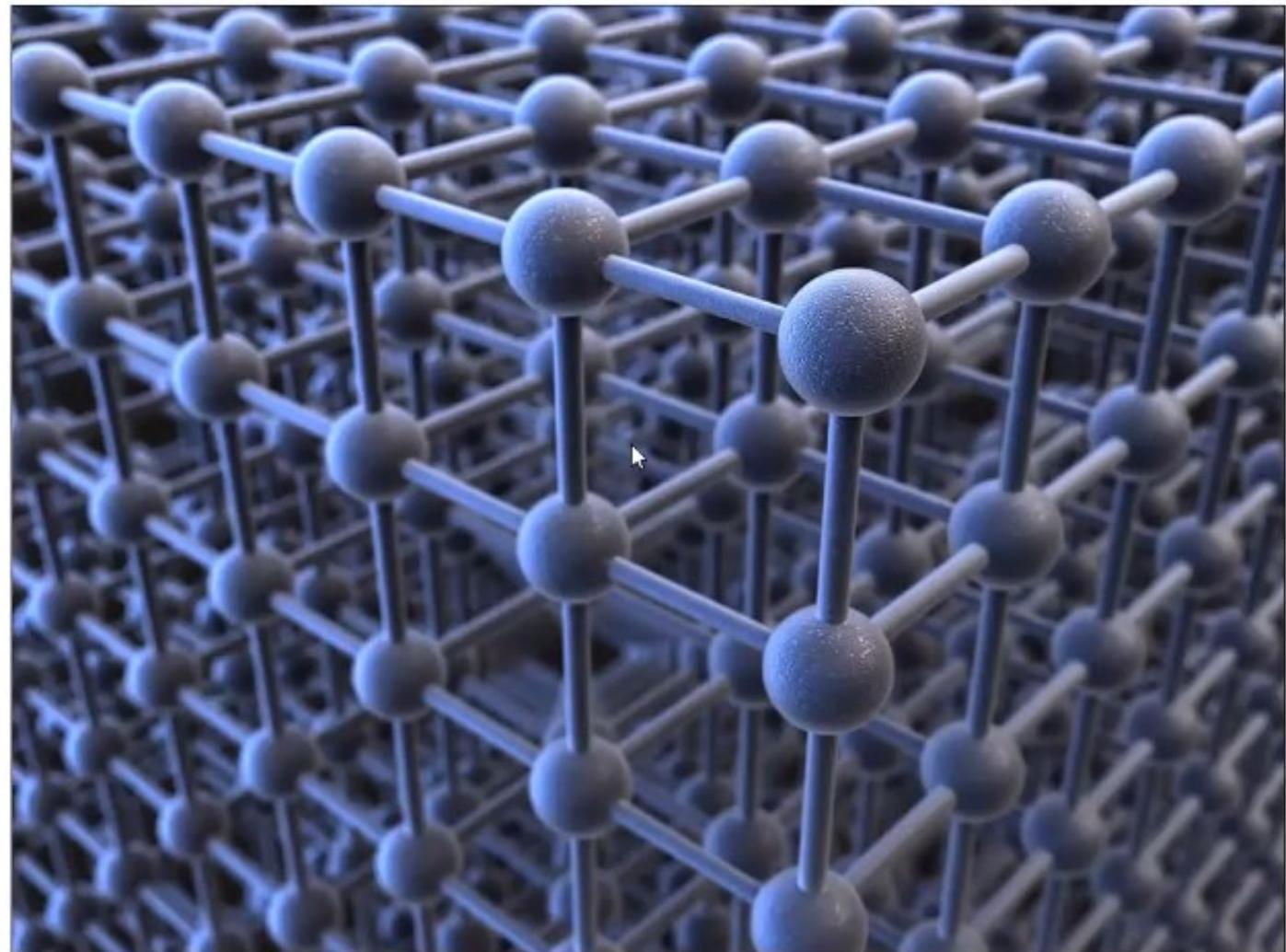


- ii. Stacking these planes on top of one another to give crystals



METALLIC CRYSTAL STRUCTURES

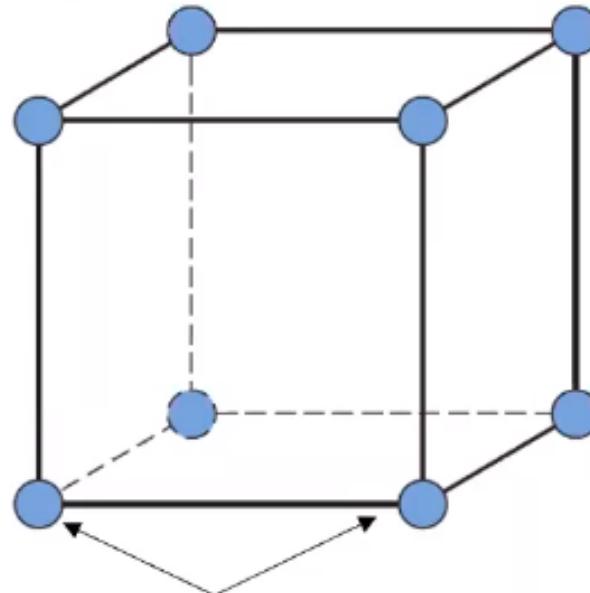
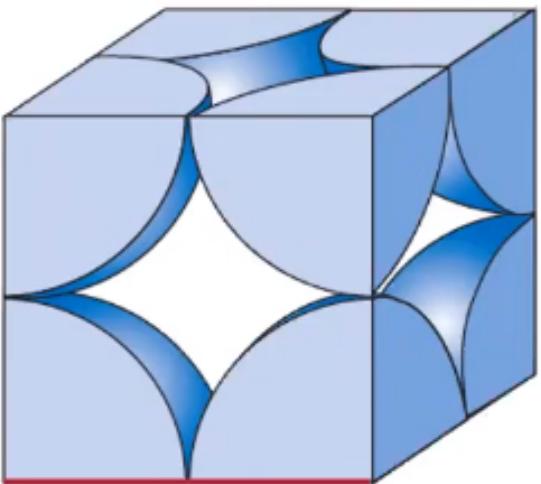
- Metals consist of regular crystal structures that form **repeating patterns** in three dimensions.
- Each **unit cell** can be regarded as the basic building block of a metal crystal.
- Like bricks, this basic structure repeats itself in three dimensions to form the metal's **crystal structure**.



Simple cubic crystal structure

METALLIC CRYSTAL STRUCTURES

SIMPLE CUBIC STRUCTURE:



Positions occupied by the centres of the atoms

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

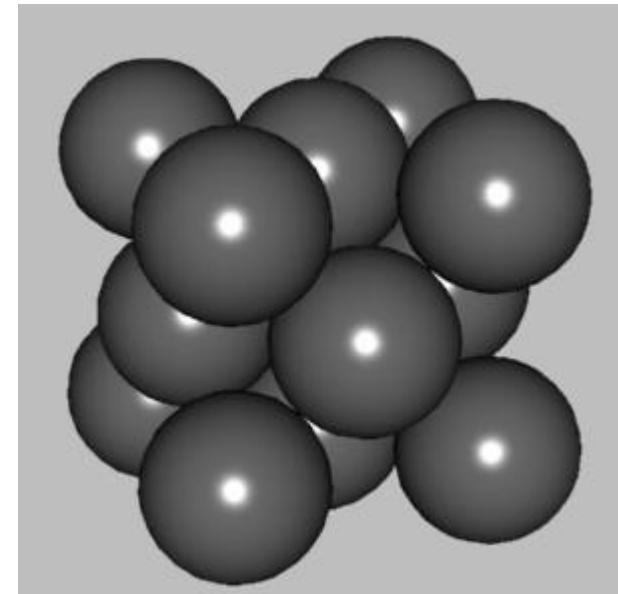
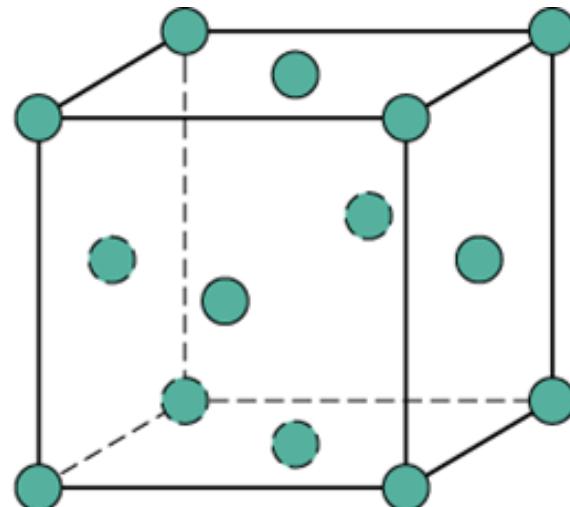
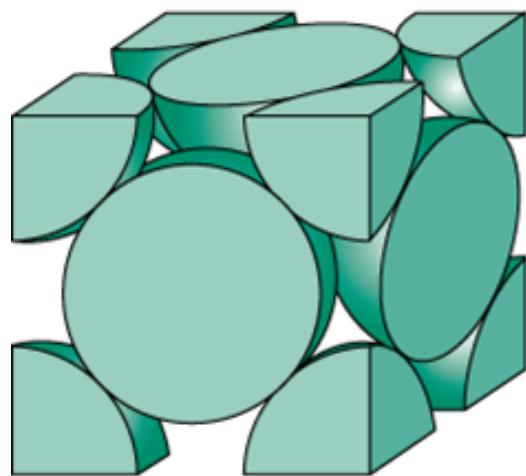
$$\boxed{APF = 0.52}$$

One equivalent atom in the unit cell ($8 \times \frac{1}{8}$)

- Rare due to low packing density (only polonium has this structure).
- **Close-packed planes** are the sides of the cube.

Face-centered cubic (FCC) Structure

Close packed directions are face diagonals



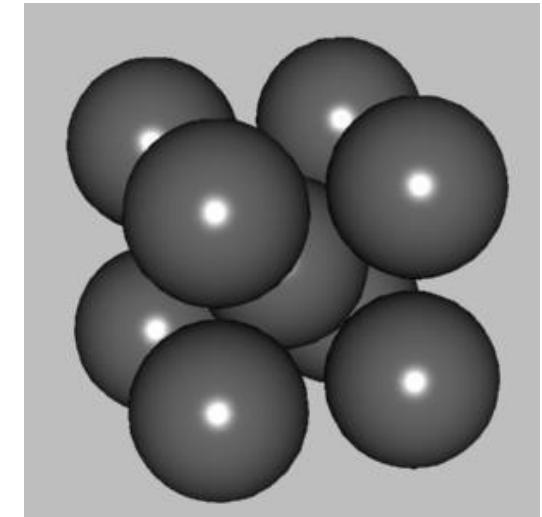
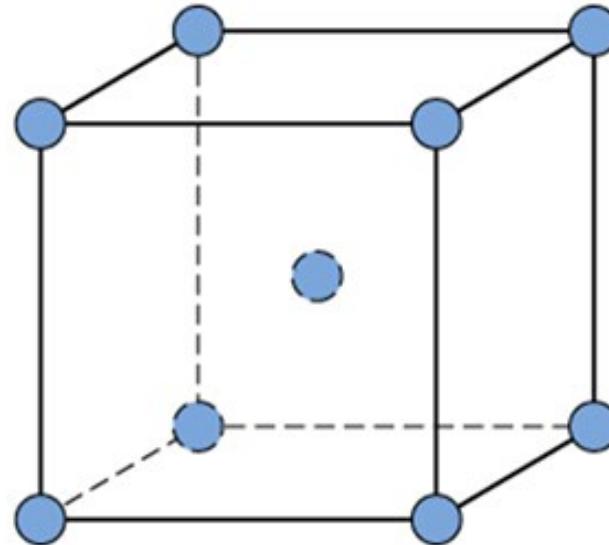
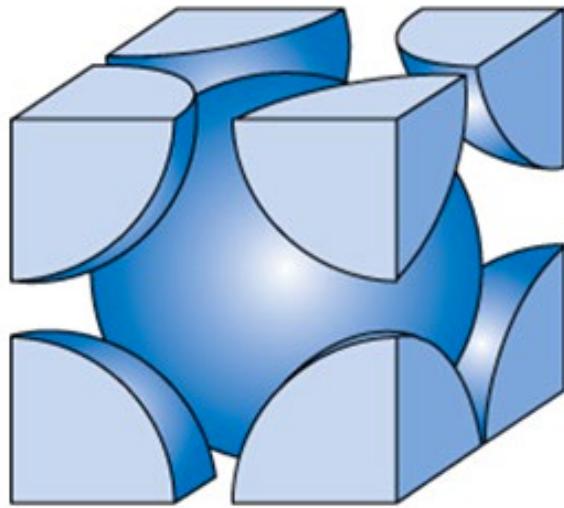
Examples: Aluminium, Copper, Nickel

Note: cube has no physical significance but merely a constructional device, called a unit cell.



Body centered cubic structure (BCC)

Close packed directions are cube diagonals, but no close-packed planes.



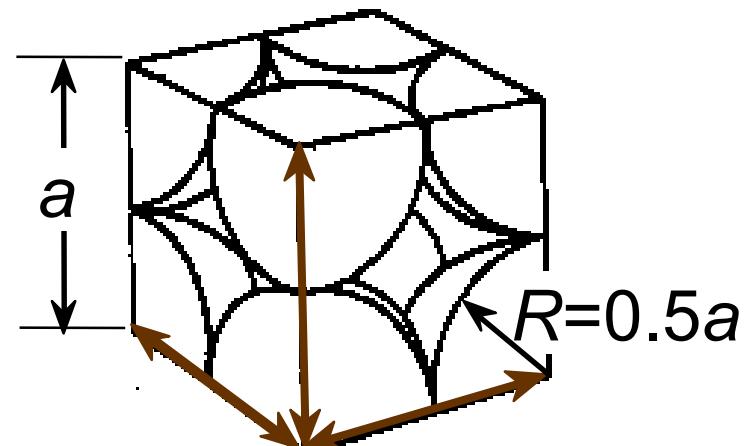
- Result is that BCC packing is less dense than FCC
- Examples: Tungsten, chromium, iron and many steels

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 $8 \times 1/8 =$

1 atom/unit cell

Adapted from Fig. 3.24,
Callister & Rethwisch 8e.

$$APF = \frac{\frac{\text{atoms}}{\text{unit cell}} \times \frac{4}{3} \pi (0.5a)^3}{a^3}$$

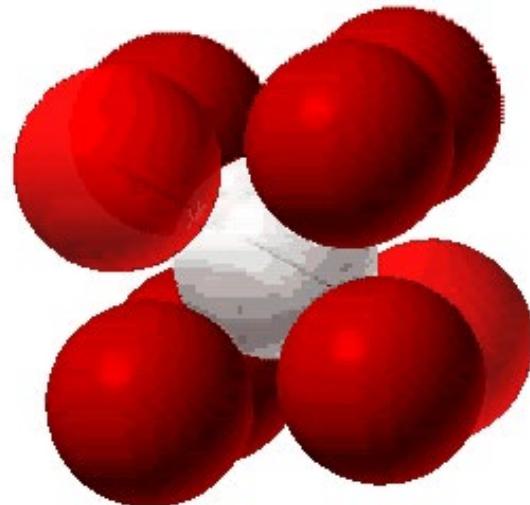
The equation is shown with annotations: 'atoms / unit cell' points to the green box containing '1'; 'volume / atom' points to the orange box containing the term $\frac{4}{3} \pi (0.5a)^3$; 'volume / unit cell' points to the blue box containing a^3 .



Body Centered Cubic Structure (BCC)

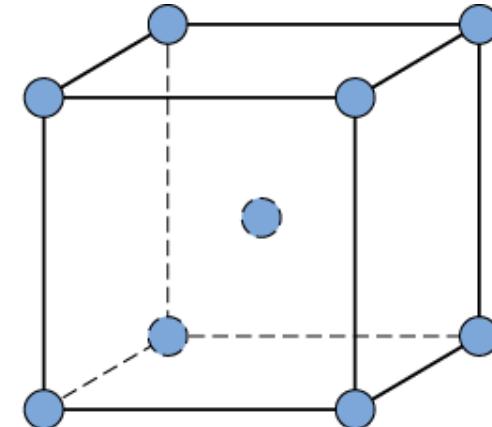
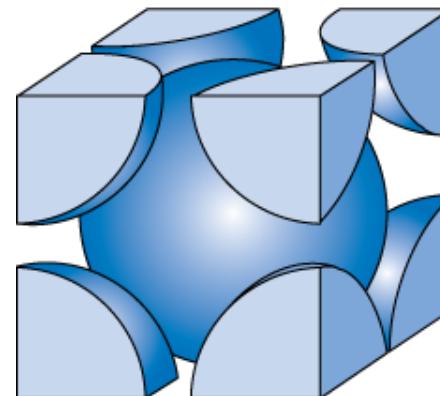
- Atoms touch each other along cube diagonals.
 - Note: All atoms are identical; the center atom is shaded differently only for ease of viewing.
- ex: Chromium, Tungsten , Iron (α), Tantalum

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



Click once on image to start animation

(Courtesy P.M. Anderson)

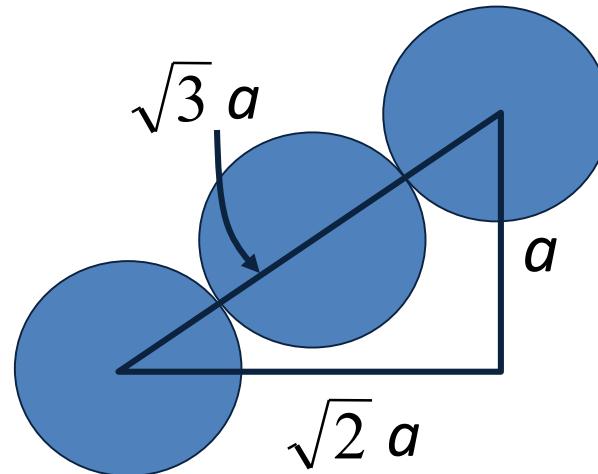
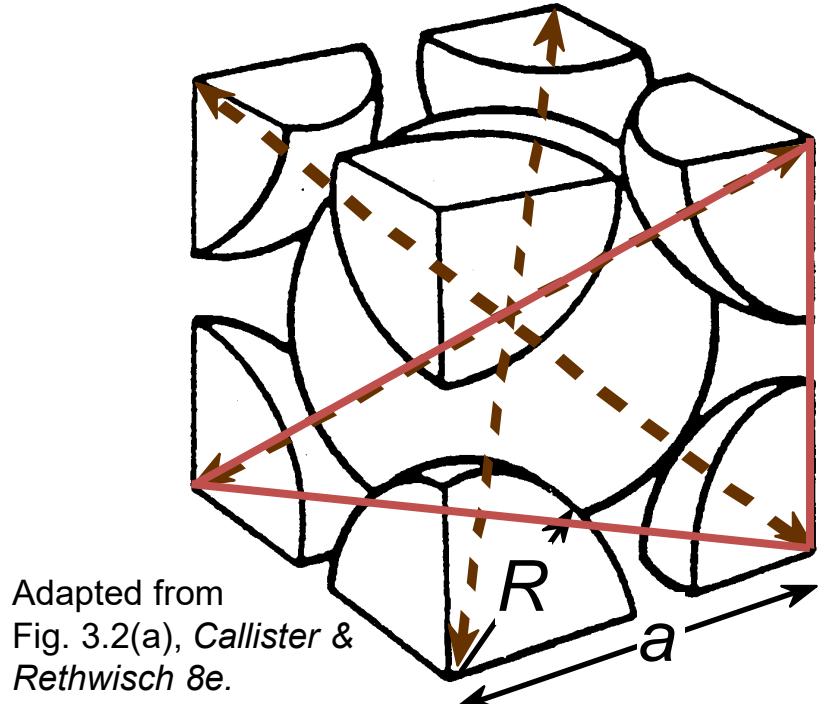


Adapted from Fig. 3.2,
Callister & Rethwisch 8e.



Atomic Packing Factor: BCC

- APF for a body-centered cubic structure = 0.68



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

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

The equation shows the calculation of the Atomic Packing Factor (APF) for a BCC structure. The numerator consists of the number of atoms per unit cell (2) multiplied by the volume of two atoms ($\frac{4}{3} \pi (\sqrt{3}a/4)^3$). The denominator consists of the volume of the unit cell (a^3) divided by the volume of one atom.

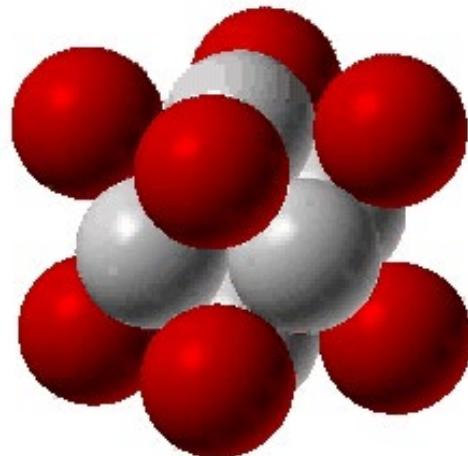


Face Centered Cubic Structure (FCC)

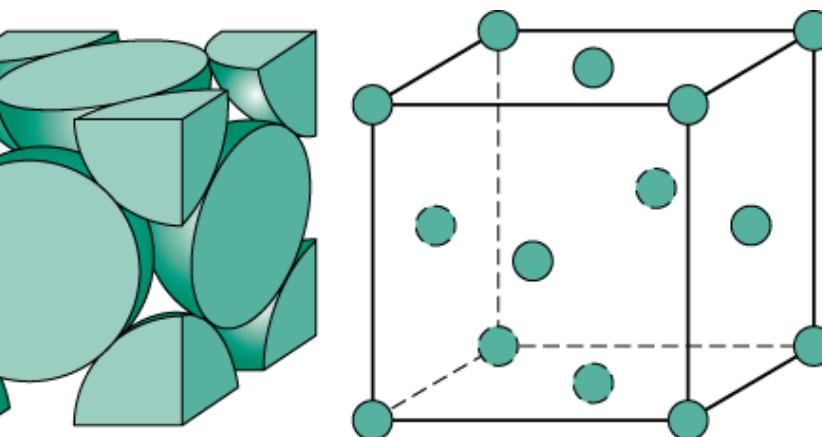
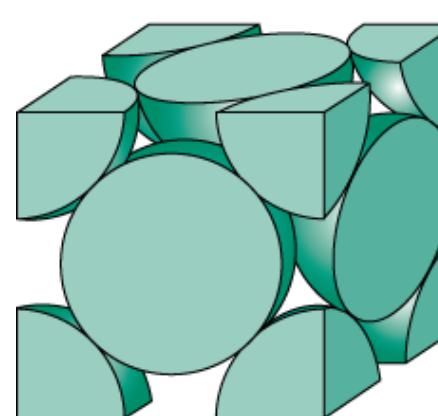
- Atoms touch each other along face diagonals.
--Note: All atoms are identical; the face-centered atoms are shaded differently only for ease of viewing.

ex: Aluminum , Copper, Gold, Lead , Nickel , Platinum , Silver

4 atoms/unit cell: $6 \text{ face} \times 1/2 + 8 \text{ corners} \times 1/8$



Click once on image to start animation
(Courtesy P.M. Anderson)



Adapted from Fig. 3.1, Callister & Rethwisch 8e.



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

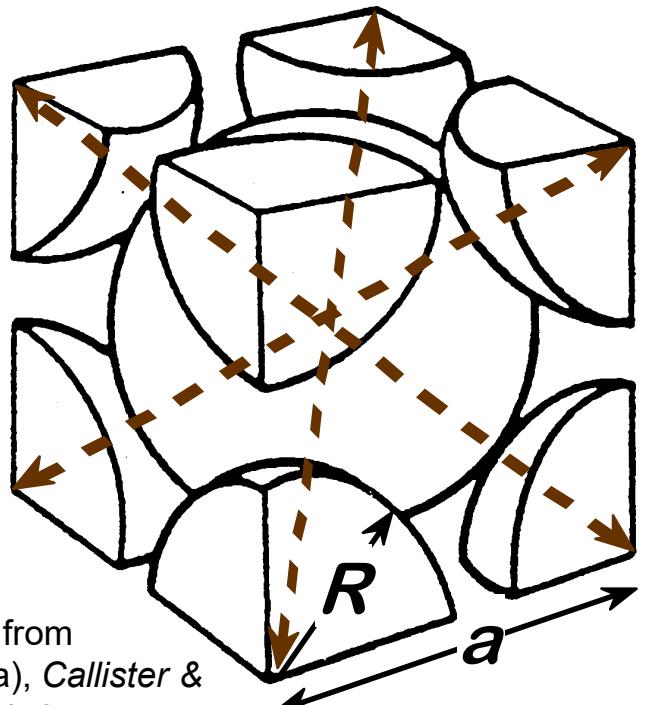
N_A = Avogadro's number

= 6.022×10^{23} atoms/mol

number of units in
one mole
of any substance



Theoretical Density, ρ



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

- Ex: Chromium Cr (BCC)

$$A = 52.00 \text{ g/mol}$$

$$R = 0.125 \text{ nm} \quad (\text{nano} = 10^{-9})$$

$$n = 2 \text{ atoms/unit cell}$$

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

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

Legend:
atoms / unit cell (green)
g / mol (brown)
volume / unit cell (blue)
atoms / mol (purple)

$\rho_{\text{theoretical}}$	$= 7.18 \text{ g/cm}^3$
ρ_{actual}	$= 7.19 \text{ g/cm}^3$



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...

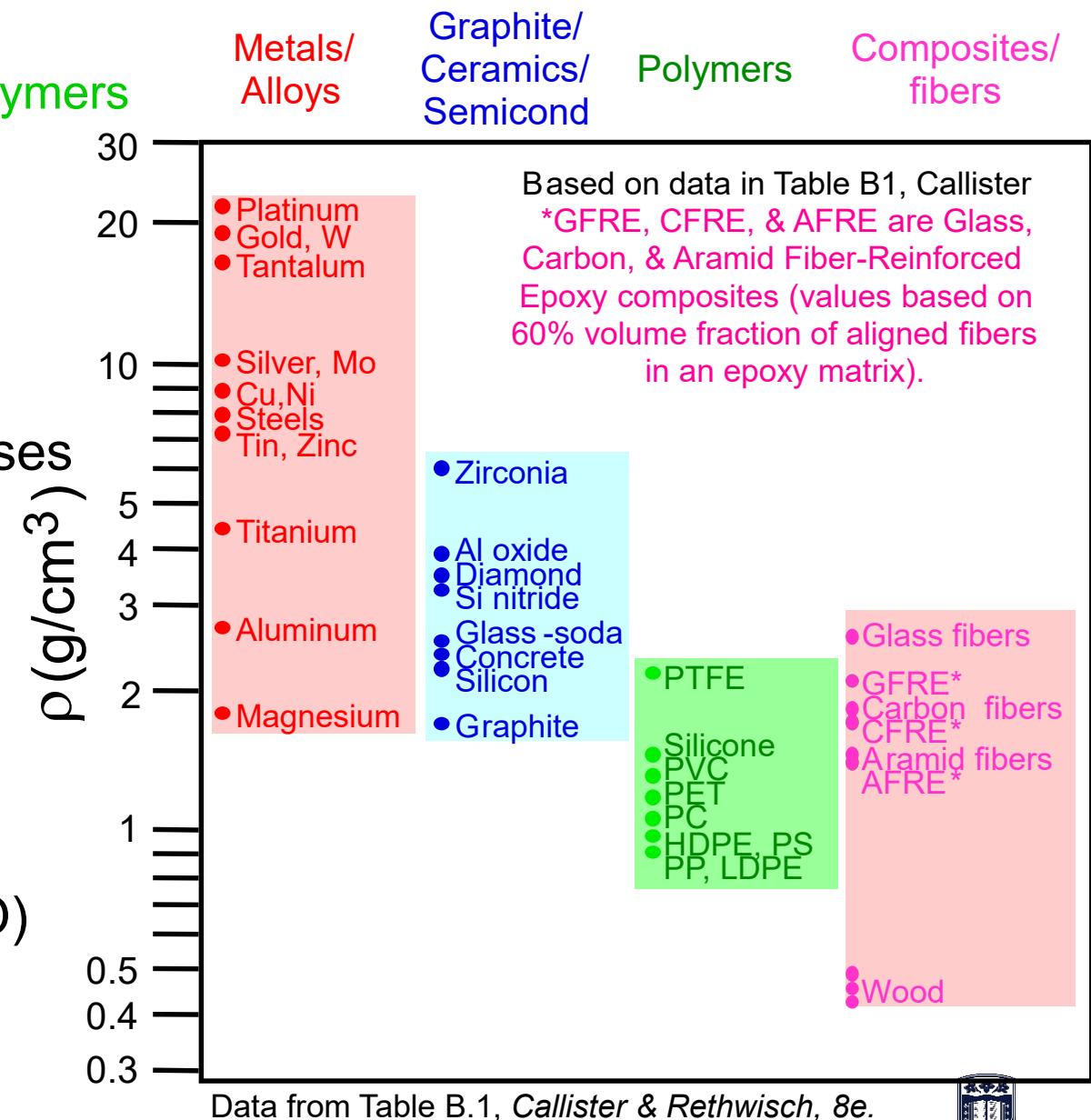
- less dense packing
- often lighter elements

Polymers have...

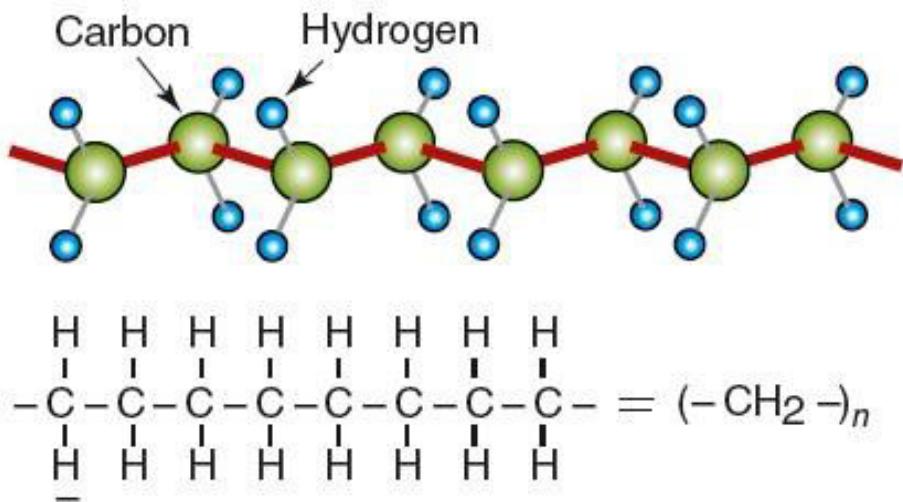
- low packing density (often amorphous)
- lighter elements (C,H,O)

Composites have...

- intermediate values



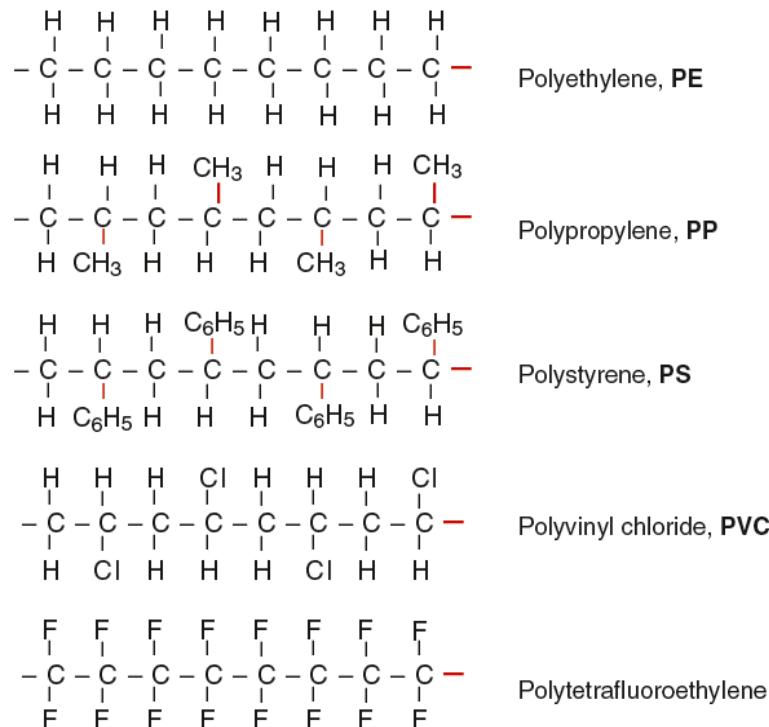
Atomic Packing in Polymers



- Polymers have a carbon-carbon backbone with varying side-groups
- Linked by covalent bonds
- Much more complex than metals
- Special mechanical properties

For background information only at this stage

We shall return to this when we study polymers in more detail later in the course



Imperfections in Solids

There is no such thing as a perfect crystal.

- What are these imperfections?
- Why are they important?

Many of the important properties of materials are due to the presence of imperfections.

For example, the mechanical properties of pure metals experience significant alterations when the metals are alloyed (i.e., when impurity atoms are added)
—for example, brass (70% copper/30% zinc) is much harder and stronger than pure copper



Types of Imperfections

- Vacancy atoms
- Interstitial atoms
- Substitutional atoms
- Dislocations
- Grain Boundaries

Point defects

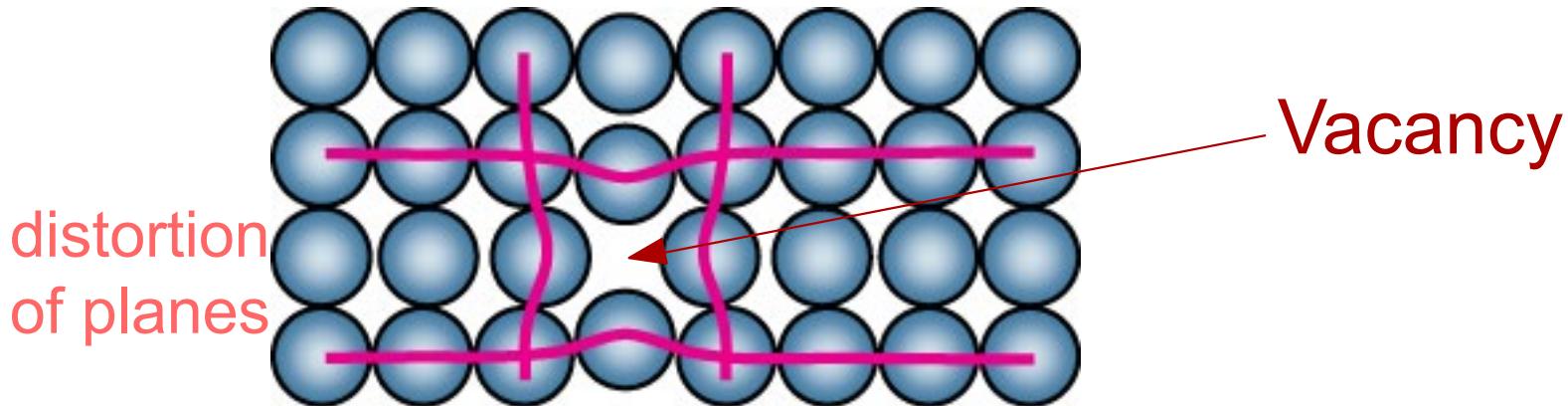
Line defects

Area defects

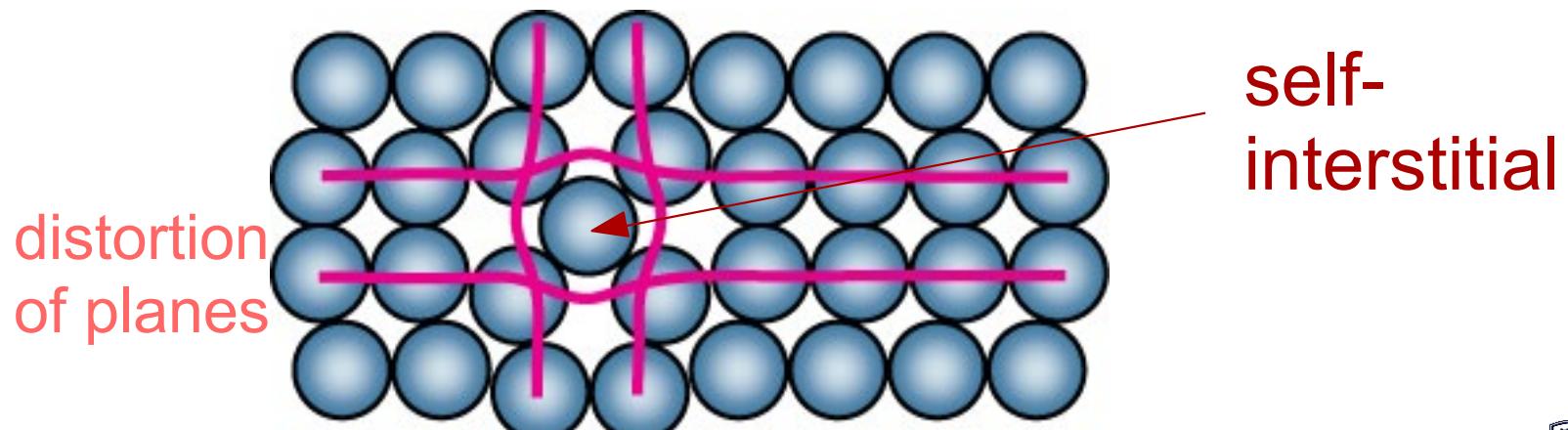


Point Defects in Metals

- **Vacancies:**
-vacant atomic sites in a structure.



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



Equilibrium Concentration : Vacancies

- varies with temperature!
- Each lattice site is a potential vacancy site

$$\frac{N_V}{N} = \exp\left(\frac{-Q_V}{k T}\right)$$

Where:

N_V – number of defects (vacancies)

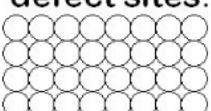
N – total number of atomic sites

Q_V – activation energy (eV)

T – temperature (Kelvin)

k_B – Boltzmann's constant
(relates temperature to energy)

No. of potential defect sites.



Each lattice site is a potential vacancy site

$$k_B = 1.38 \times 10^{-23} \text{ J/atom K}$$
$$= 8.62 \times 10^{-5} \text{ eV/atom K}$$

$$1 \text{ eV} = 1.602 \times 10^{-19} \text{ J}$$

$$N = (\rho) \left(\frac{N_A}{A} \right)$$

Where:

N – number of sites

ρ – density

A – Atomic mass

N_A – Avogadro number

$(6.022 \times 10^{23} \text{ atom/mol})$

(number of units in one mole of any substance)

(The units may be electrons, atoms, ions, or molecules)



Example 3.1

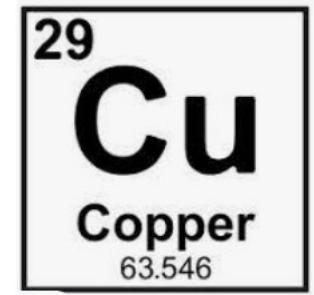
Let's estimate the number of vacancies in copper (Cu) at room Temperature

$$N_v = N_s \exp\left(-\frac{Q_v}{k_B T}\right)$$

The Boltzmann's constant

$$k_B = 1.38 \times 10^{-23} \text{ (J/atom-K)} \\ = 8.62 \times 10^{-5} \text{ (eV/atom-K)}$$

The energy for vacancy formation $Q_v = 0.9 \text{ eV/atom}$



Given:

$$N_A = 6.022 \times 10^{23} \text{ atoms/mol}$$

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

$$A_{cu} = 63.5 \text{ g/mol}$$



Example 3.1

Let's estimate the number of vacancies in copper (Cu) at **room Temperature (27°C)**

$$N_v = N_s \exp\left(-\frac{Q_v}{k_B T}\right)$$

The Boltzmann's constant

$$k_B = 1.38 \times 10^{-23} \text{ (J/atom-K)} \\ = 8.62 \times 10^{-5} \text{ (eV/atom-K)}$$

The temperature in Kelvin $T = 27^\circ\text{C} + 273 = 300 \text{ K}$.

$$k_B(T) = 300 \text{ K} \times 8.62 \times 10^{-5} \text{ (eV/K)} = 0.02586 \text{ eV}$$

The energy for vacancy formation $Q_v = 0.9 \text{ eV/atom}$

The number of regular lattice sites $N_s = (N_A)(\rho)/A_{\text{cu}}$

$$\frac{N_V}{N} = \exp\left(\frac{-Q_v}{k_B T}\right)$$

$$N_V = (8.42 \times 10^{22}) \exp\left(\frac{-0.9}{(0.02586)}\right)$$

$$N_V = 6.4 \times 10^7 \text{ vacancies per cm}^3$$

Given:

$$N_A = 6.022 \times 10^{23} \text{ atoms/mol}$$

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

$$A_{\text{cu}} = 63.5 \text{ g/mol}$$

$$N = (\rho) \left(\frac{N_A}{A} \right)$$

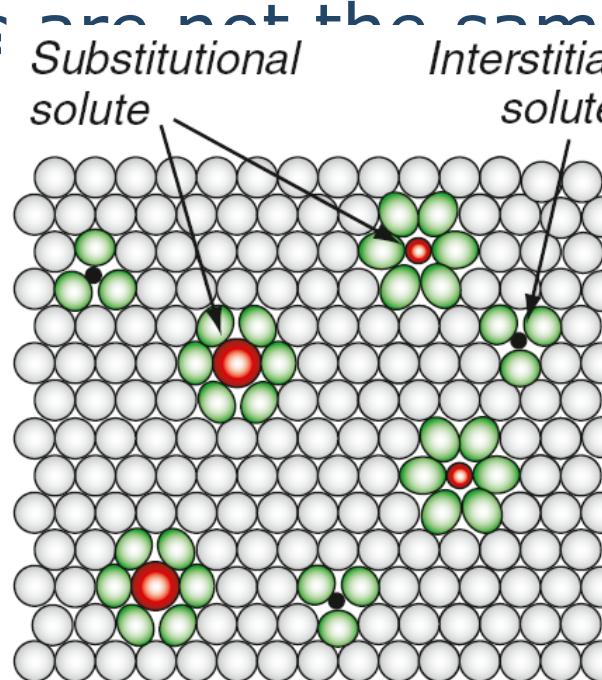
$$N = (8.89) \left(\frac{6.022 \times 10^{23}}{63.5} \right)$$

$$N = 8.42 \times 10^{22} \text{ atom/cm}^3$$



Point defects: Solute Atoms

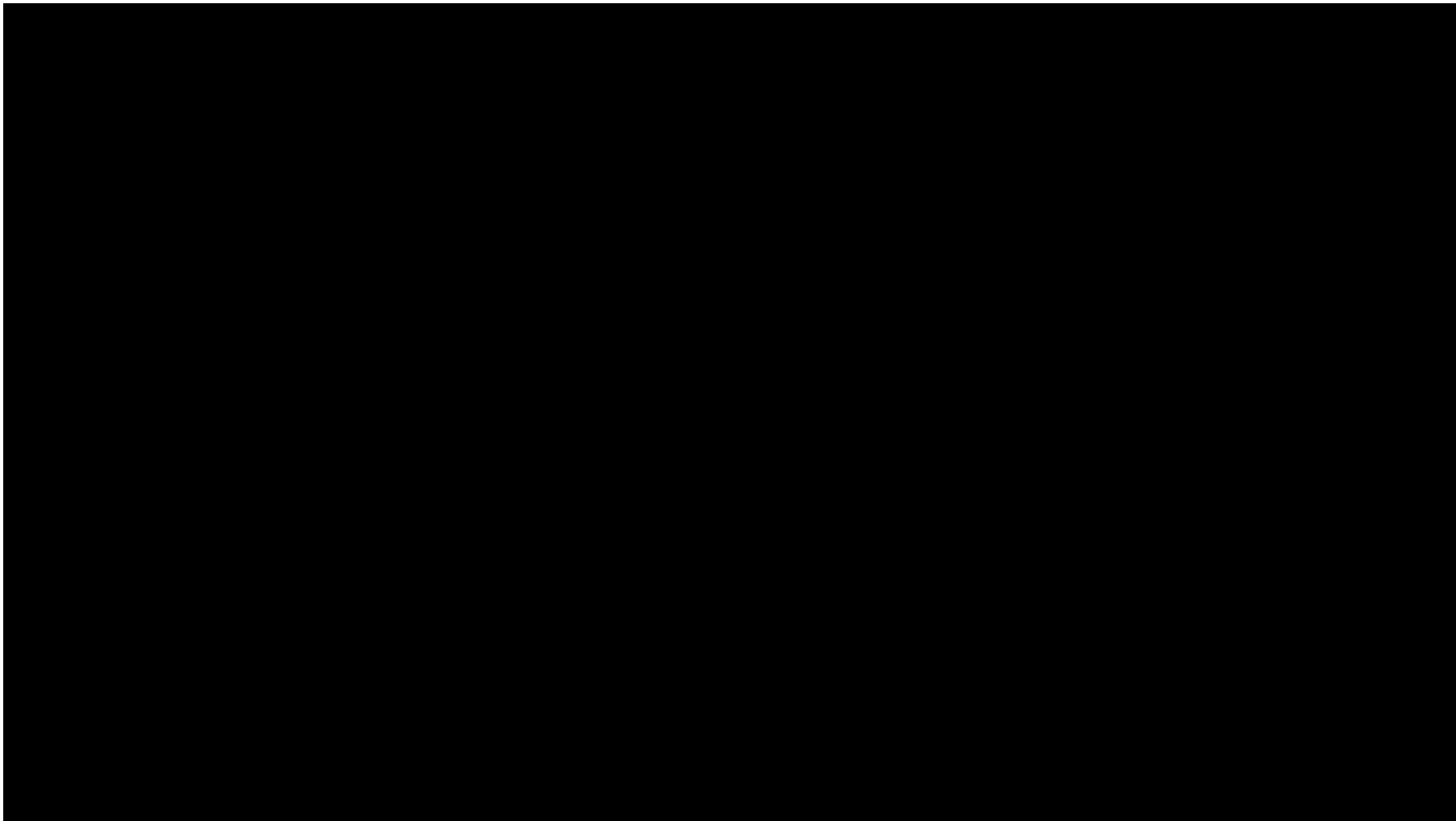
- Substitutional:
 - Solute (impurity) atom replaces a host atom.
- Interstitial:
 - Solute (impurity) atom occupies an interstitial site in the lattice.
- Solute atoms ~~are not the same~~ size so distort the lattice.



Stop and check video on moodle

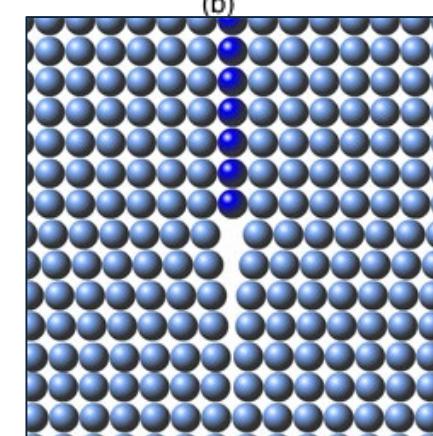
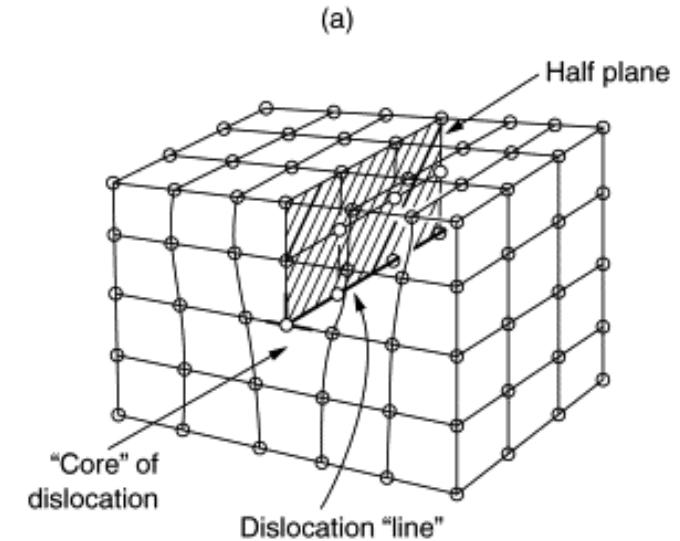
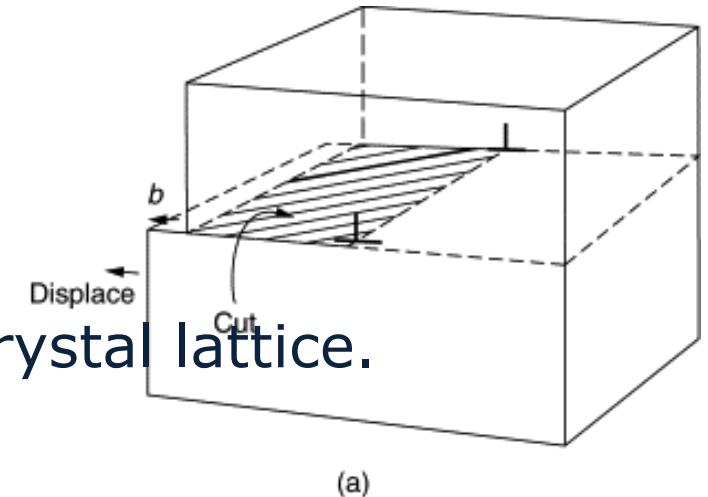
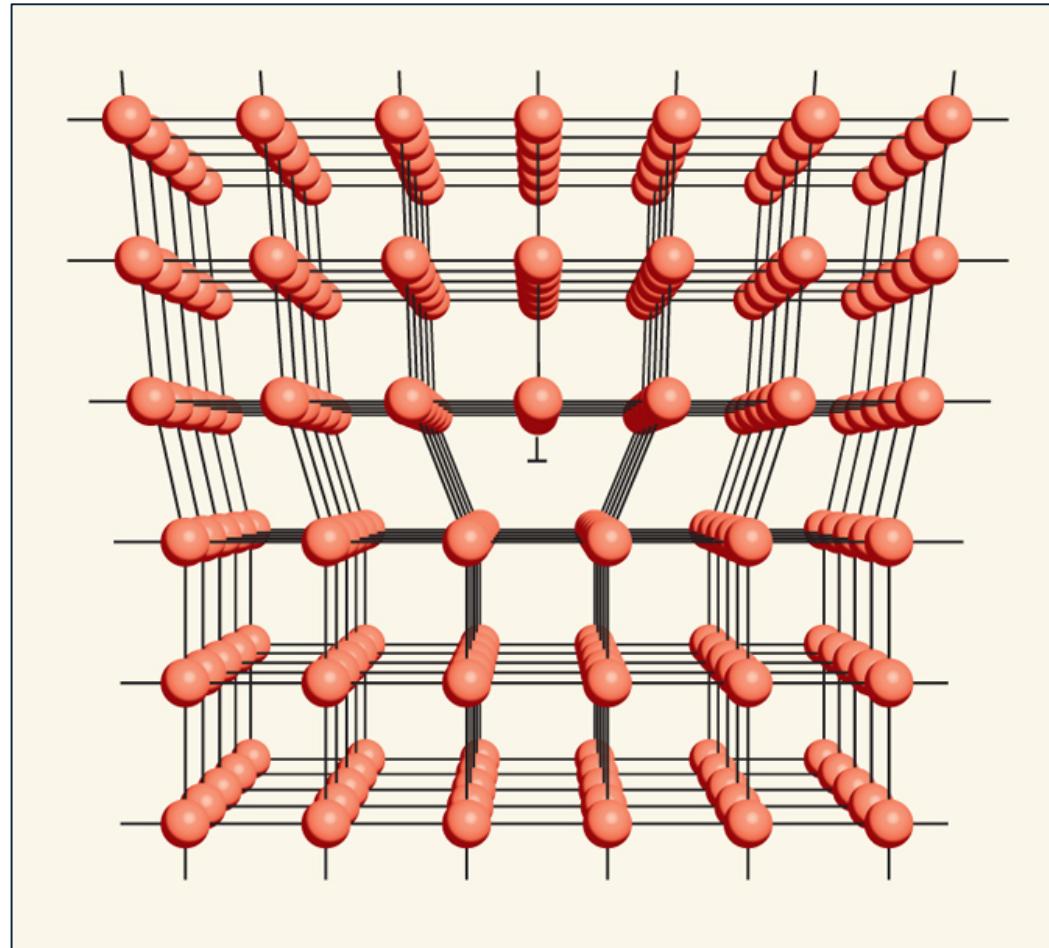


Lecture 1: Stop and Check Video



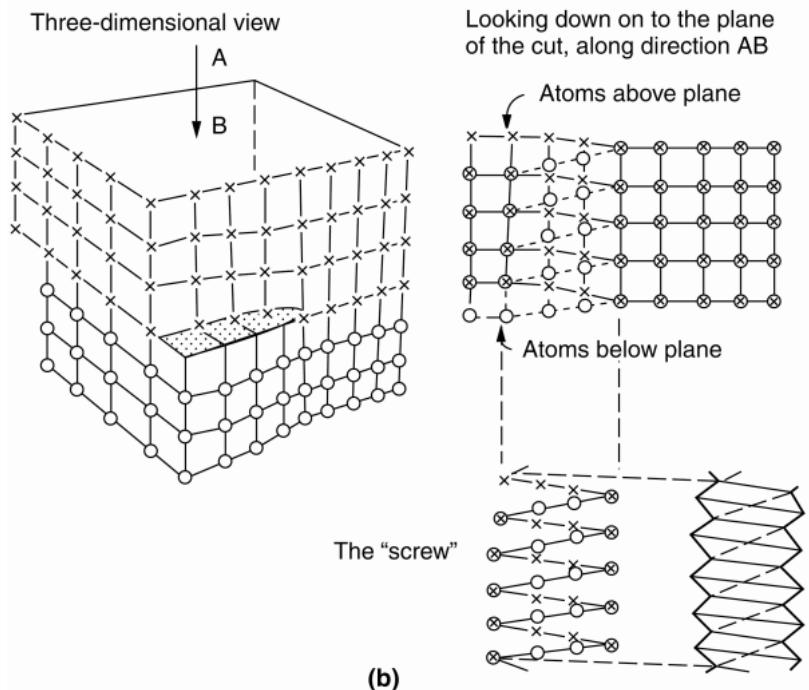
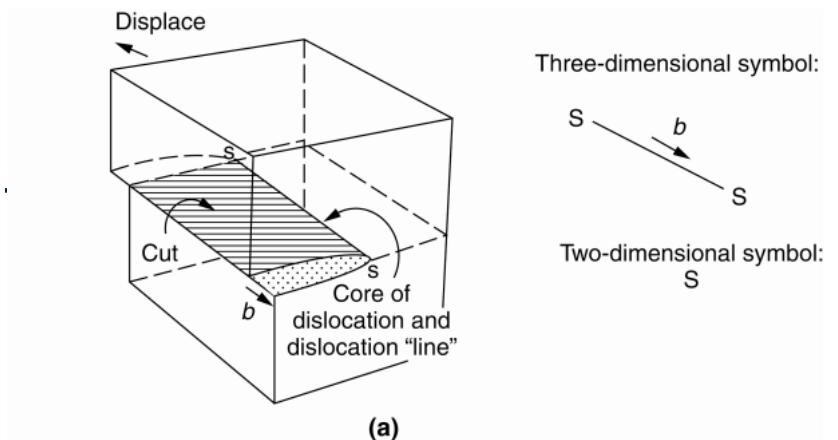
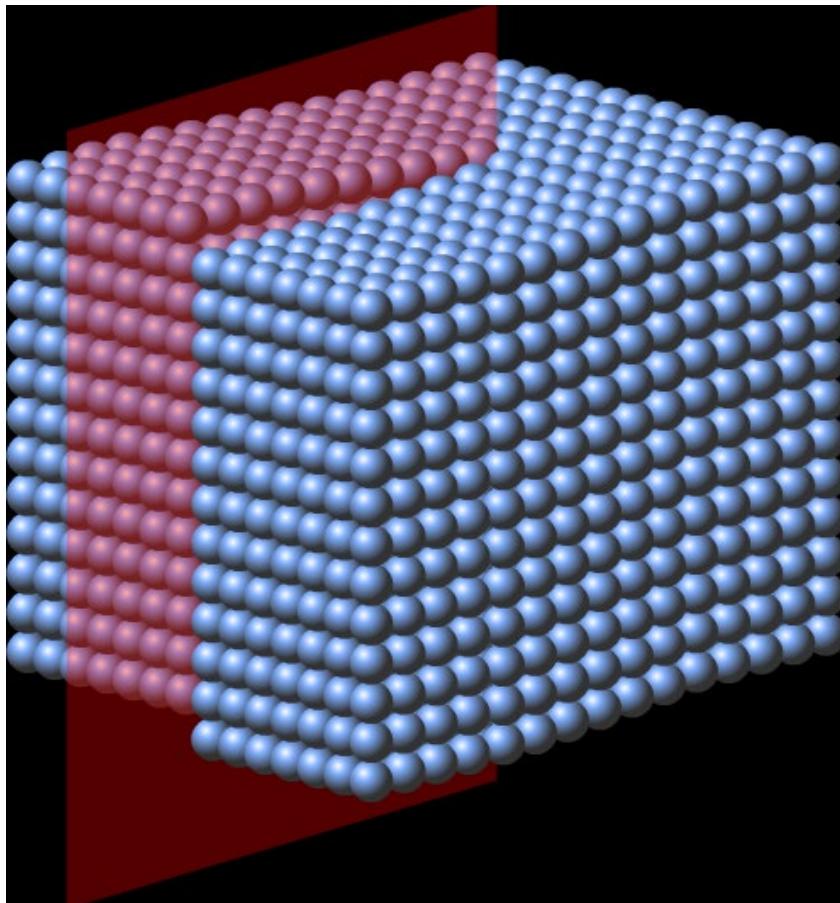
Line defects: Dislocations

- Edge dislocation:
 - Extra half plane of atoms in the crystal lattice.



Line defects: Dislocations

- Screw dislocation:
 - Acts to distort atom planes in a screw-like motion



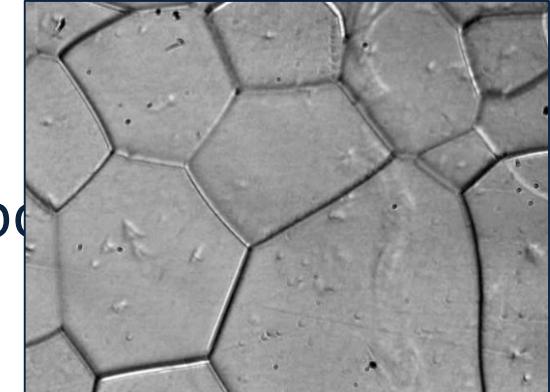
Dislocation

- The dislocations move along the densest planes of atoms in a material, because the stress needed to move the dislocation increases with the spacing between the planes.
- FCC and BCC metals have many dense planes, so dislocations move relatively easy and these materials have high ductility.
- Metals are strengthened by making it more difficult for dislocations to move.
- This may involve the introduction of obstacles, such as interstitial atoms or grain boundaries, to “pin” the dislocations.
- Also, as a material plastically deforms, more dislocations are produced and they will get into each others way and impede movement. This is why strain or work hardening occurs.

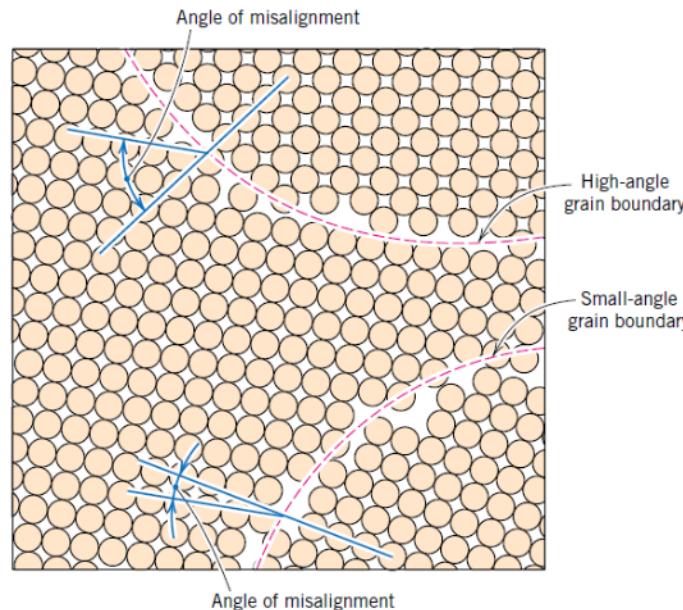
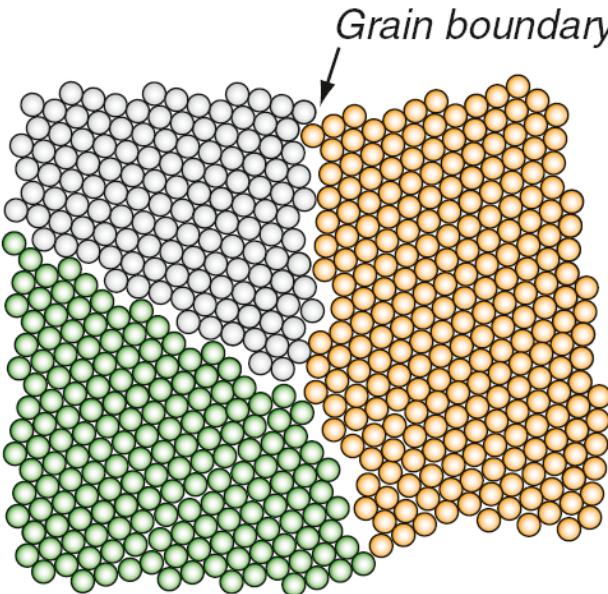


Area Defects

Grain boundaries

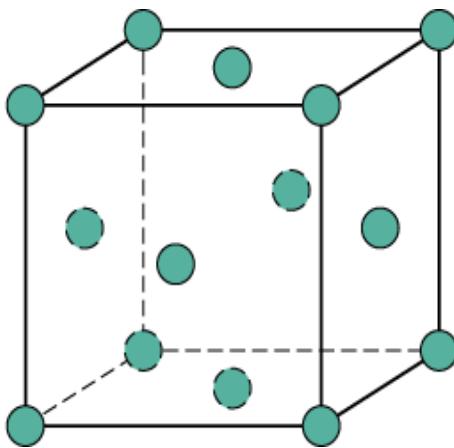
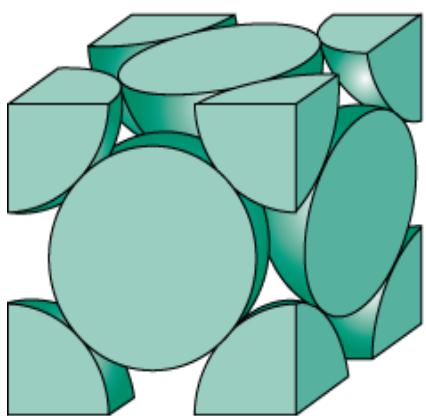


- Free surfaces:
 - Atoms at the free surface are not fully bonded.
- Grain boundaries:
 - Boundaries between crystals of different orientations.
 - Individual crystals are called 'grains'.
 - More grain boundaries means higher resistance to slip.
 - More grains means more uniform the mechanical properties

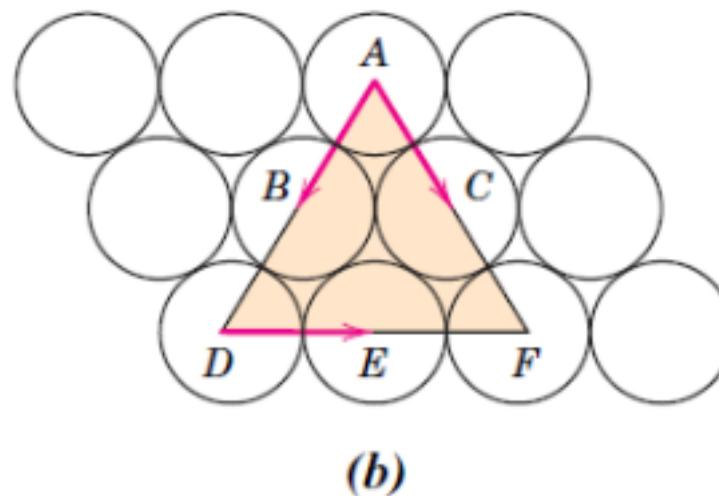
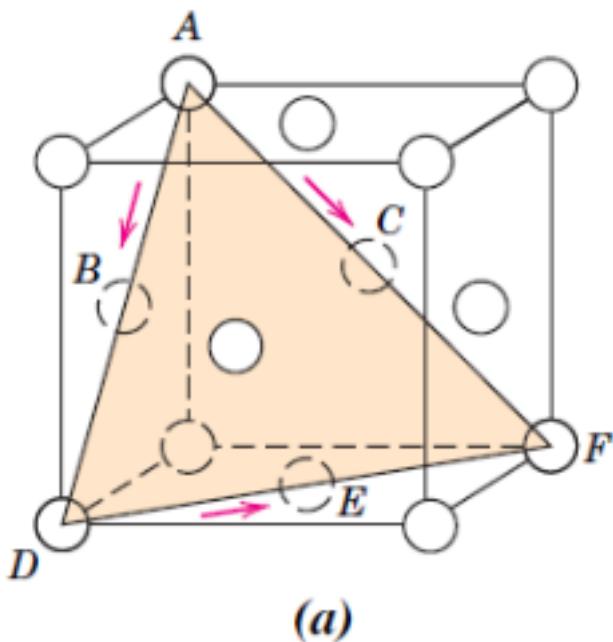


optical microscopy, the light microscope is used to study the microstructure

Slip systems



- Slip system shown within an FCC unit cell.
- A slip plane and 3 slip directions.

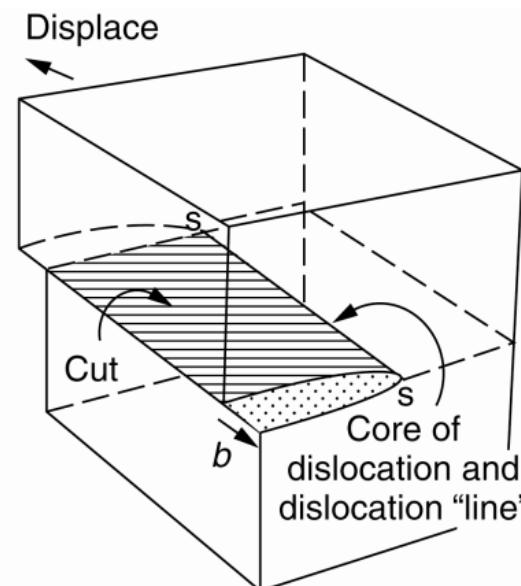
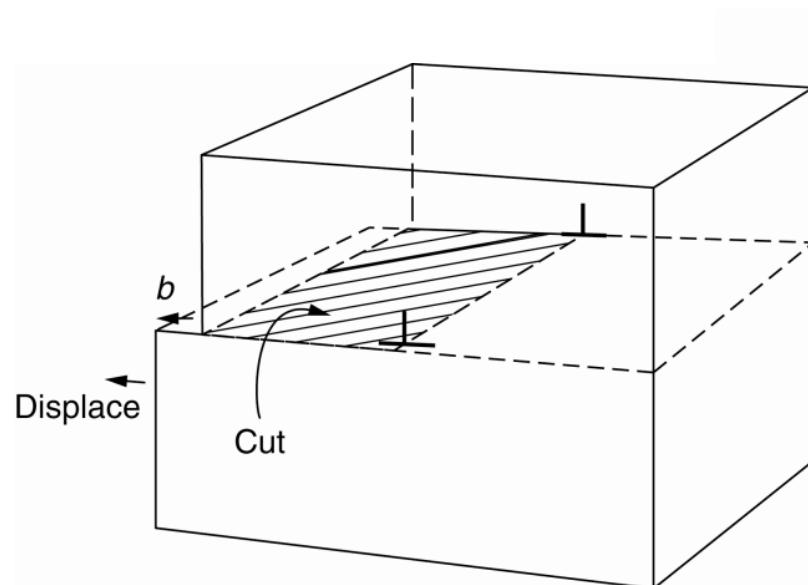


- Dislocations do not move with the same degree of ease on all crystallographic planes of atoms and in all crystallographic directions.
- Typically, there is a preferred plane, and in that plane there are specific directions along which dislocation motion occurs.



Dislocations and Plastic Deformation

- Dislocations are the key to plastic deformation in crystals.
- Dislocations are the weakest 'link' in the lattice.
- Permanent deformation occurs as dislocations move along slip planes in metals.
- Dislocations move under the influence of a *shear stress*.
 - Dislocation movement results in plastic strain.



Stop and check resources on moodle



Lecture 1: Stop and Check resources



UNIVERSITY
OF WOLLONGONG
IN DUBAI



UNIVERSITY
OF WOLLONGONG
IN DUBAI



ENGG103 Materials in Design