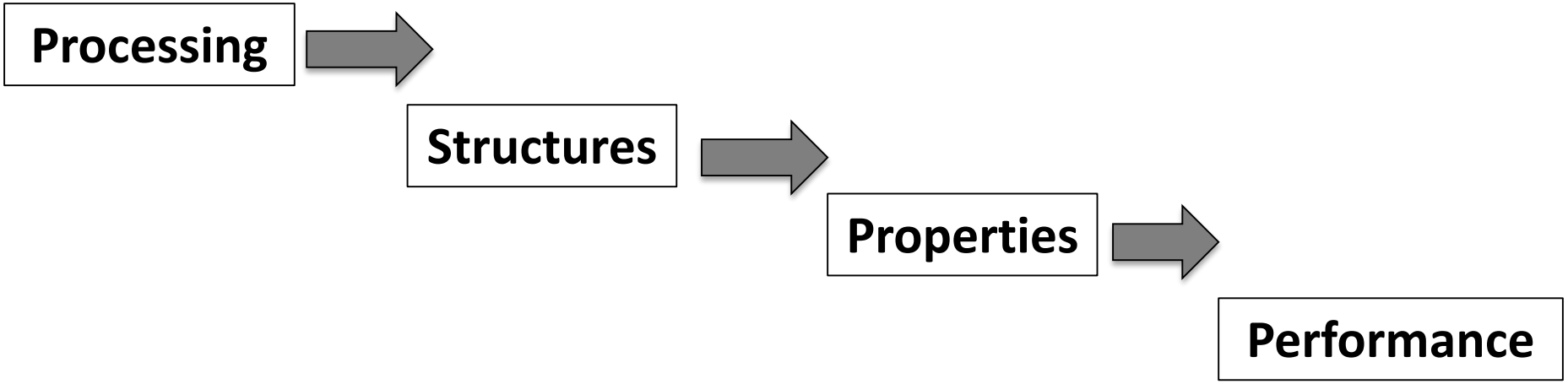
Review

Chapter 1
Introduction

Chapter 1: Summary

1) Materials Science and Engineering



2) Classification of Materials

(metals, ceramic, polymers, etc)

Classification of Materials

Metals:

Composed of one or more metallic elements, Fe, Cu, Al (& often small amounts of nonmetallic elements, O2, N2, C)

Ceramic

Compounds between metallic and nonmetallic elements (usually oxides, nitrides, carbides). Al2O3, SiC, glass, etc

Polymers

Plastic and rubbers (mainly based on carbon, hydrogen, and other nonmetallic elements.

Composites

Composed of two or more of the above classes (fiberglass, carbonfiber)

Advanced materials *(for high-tech applications)*

e.g. semiconductor, biomaterials, nano-materials, etc

Chapter 2

Atomic Structure and Interatomic Bonding

Atom

Nucleus

Proton (p^+) & neutron (n^0)

1.6×10^{-9} C
1.673×10^{-27} kg

Electron (e^-)

-1.6×10^{-9} C
9.11×10^{-31} kg

$^{A}_{Z}X$

Atomic mass = $mass_{p+} + mass_n$

Atomic number = n_p
($=n_e$ for neutral atom)

Review (from Chapter 2)

How do you calculate:

- N_{moles}: # of moles
- N_{atoms}: # of atoms

Remember that you need N_{atoms} to calculate the equilibrium number of vacancies, $N_v = N \exp(Q_v/kT)$.

Given:

- Atomic weight, A (g/mole)
- Avogadro number, N_{av} (atoms/mole)
- Mass, M (g) or density, d (g/cm^3)

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1 mole ----------> A (g/mole)

N_{moles} ----------> M (g)

➔ $N_{moles} = M / A$

---

1 mole ----------> N_{av} (atoms/mole)

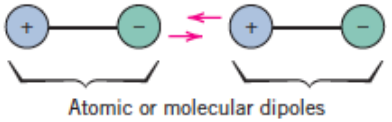
N_{moles} ----------> N_{atoms}

➔ $N_{atoms} = N_{av} * N_{moles}$ ➔ $N_{atoms} = N_{av}\, M / A$

Atomic Bonds

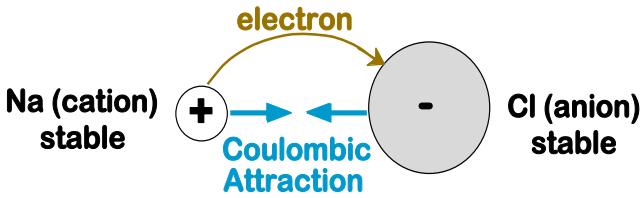
Primary interatomic bonds

Secondary, van der Waals, or physical bonds



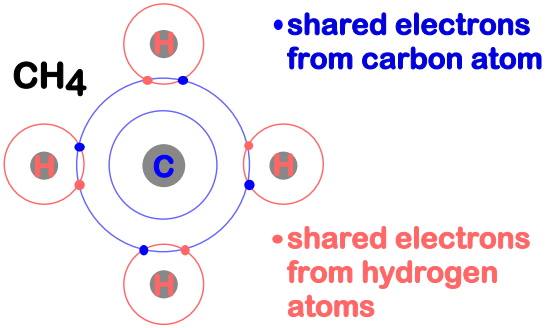
Ionic bonding

Atoms give up their valence electrons to other atoms



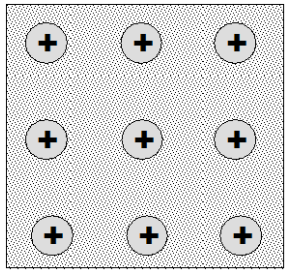
Covalent bonding

share electrons between adjacent atoms



Metallic bonding

Arises from a sea of donated valence electrons



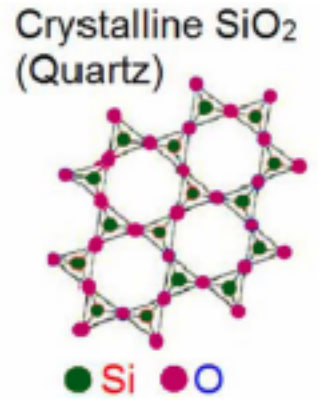
Chapter 3

The Structure of Crystalline Solids

- Crystalline vs. non-crystalline materials
- Crystal structure, crystal system, lattice, unit cell, lattice parameters
- SC, BCC, FCC, HCP
  - Close packed direction
  - Coordination # (Z)
  - # of atoms/unit cell
  - APF

- Theoretical Density
- Single crystal vs. polycrystalline materials
- Point coordinates
- **Crystal direction**
- **Crystal planes**
- Linear density, $LD_{[xxx]}$
- Planar density, $PD_{(xxx)}$

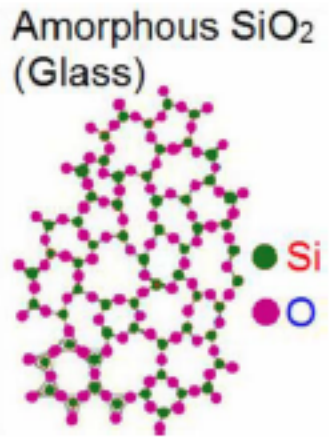
Atomic arrangement



Solid

Crystalline

Amorphous

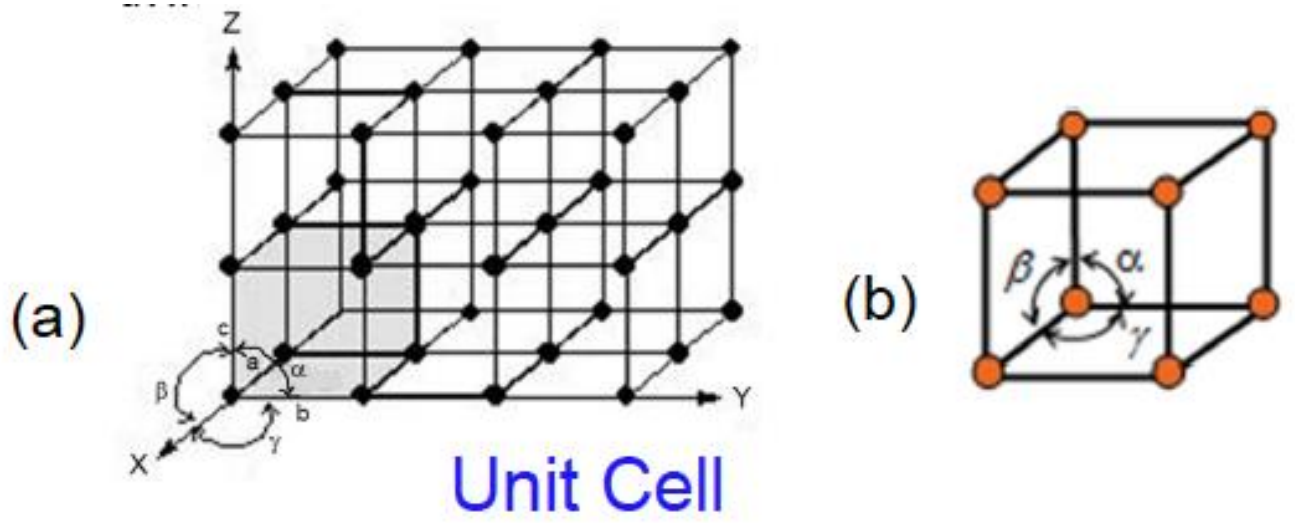


Crystalline – periodic arrangement of atoms: definite repetitive pattern

Non-crystalline or Amorphous – random arrangement of atoms.

Crystal structure

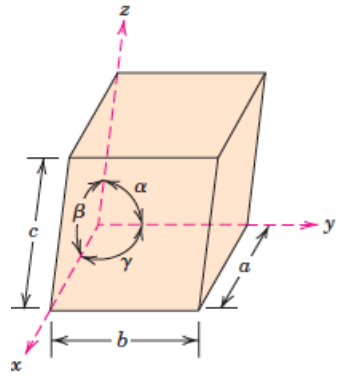
Crystal structure: spatial arrangement of atoms



Lattice: 3D array of points coinciding with atom positions *(hard sphere model)*

Unit cell: The basic structural unit of a crystal structure

Crystal system: defined based on the geometry of a unit cell (lattice parameters: a, b, c, α, β, γ)

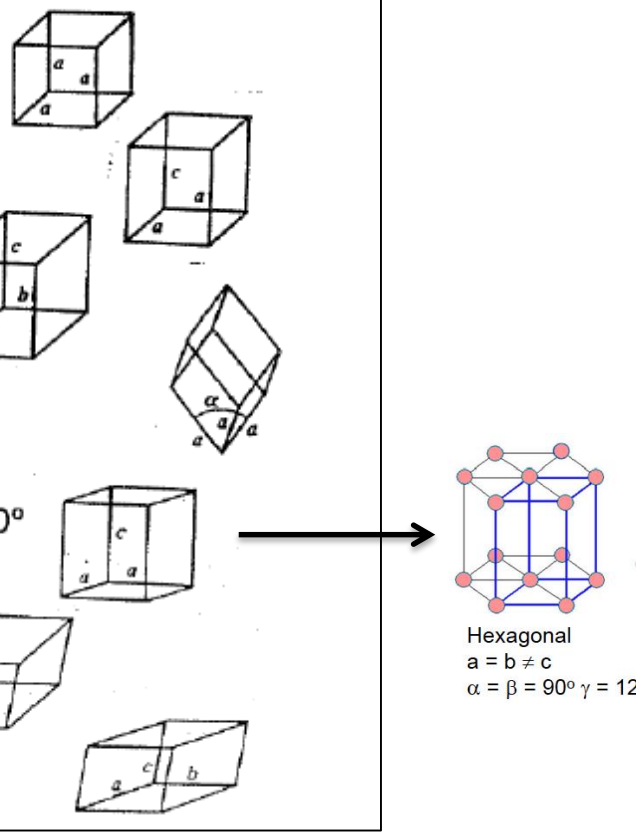


Crystal structure

- **7** Crystal systems ← 7 unique "shapes" of unit cells

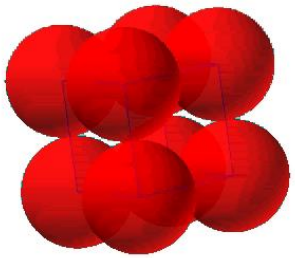
Shape of unite cell → **7** Crystal Systems

Cubic	$a=b=c,\ \alpha=\beta=\gamma=90^o$
Tetragonal	$a=b\neq c,\ \alpha=\beta=\gamma=90^o$
Orthorhombic (or Rhombic)	$a\neq b\neq c,\ \alpha=\beta=\gamma=90^o$
Rhombohedral (or Trigonal)	$a=b=c,\ \alpha=\beta=\gamma\neq 90^o$
Hexagonal	$a=b\neq c,\ \alpha=\beta=90^o,\ \gamma=120^o$
Monoclinic	$a\neq b\neq c,\ \alpha=\gamma=90^o\neq\beta$
Triclinic	$a\neq b\neq c,\ \alpha\neq\beta\neq\gamma\neq 90^o$

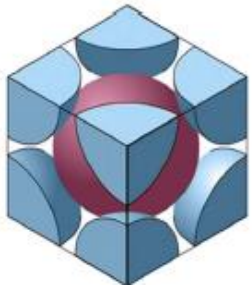


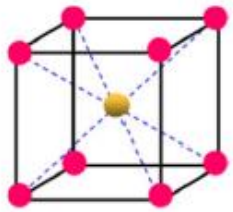
Hexagonal
a = b ≠ c
α = β = 90° γ = 12

SIMPLE CUBIC STRUCTURE (SC)

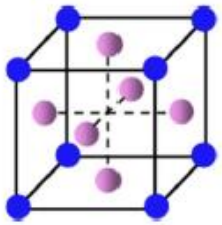


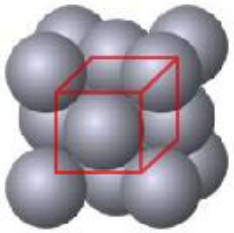
Body Centered Cubic (BCC)



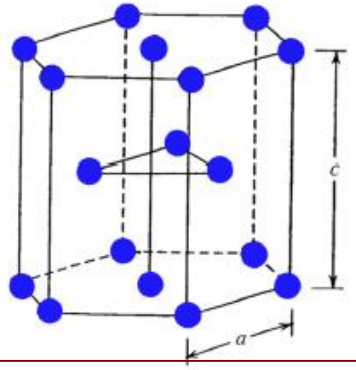


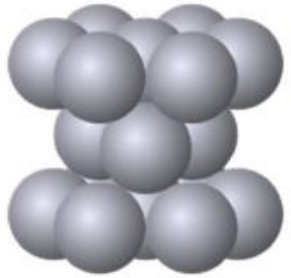
Face Centered Cubic (FCC)





Hexagonal Close Packed (HCP)





Close packed direction:

Coordination # (Z): no. of nearest neighbor to a a particular atom in the crystal

# of atoms/unit cell:

Atomic Packing Factor =

$$\text{APF} = \frac{\text{volume of atoms in a unit cell}}{\text{total unit cell volume}}$$

	Close packed direction	Coordination # (Z)	# of atoms/unit cell	APF
Simple cubic	Cube edge	6	1	0.52
Body Centered Cubic (BCC)	Cube 0.68 diagonal	8	2	
Face Centered Cubic (FCC)	Face Diagonal	12	4	0.74
Hexagonal Close Packed	Edge	12	6	0.74

THEORETICAL DENSITY

$$r = \frac{n A}{V_c N_A}$$

- n: # atoms/unit cell
- A: Atomic weight (g/mol)
- V_c: Volume/unit cell (cm^3/unit cell)
- N_A: Avogadro's number (6.023×10^{23} atoms/mol)

Example: Copper

- 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)

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

Result: theoretical $r_{Cu} = 8.89$ g/cm^3
Compare to actual: $r_{Cu} = 8.94$ g/cm^3

❑ Crystallographic direction

To specify a direction:

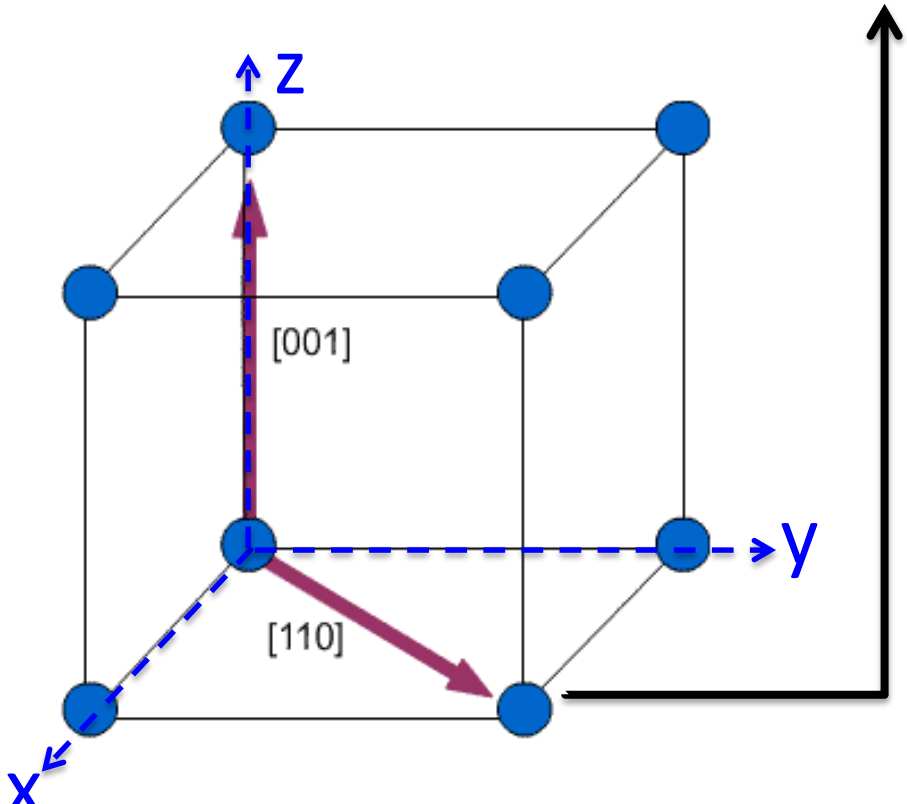
Position the vector such that it passes through the origin

1. Find the coordinates of the two ends of the line (head & tail)
2. Subtract the coordinates of the two ends (head-tail)
3. Convert fractions, if any, into integers (multiply by a common factor) and reduce to lowest terms
4. Enclose in square brackets [u v w]

Coordinates of Head:	1	1	0
Coordinates of Tail:	0	0	0
Subtract:	1	1	0

No fractions

=> [u v w] = [1 1 0]

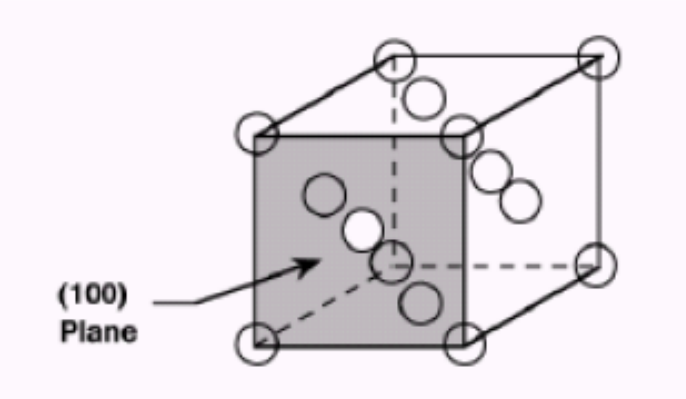


❑ Crystallographic Planes:

Planes are described by notations, called **Miller indices (h k l)**

To find the Miller Indices of a plane, follow these steps:

- Determine the intercepts of the plane along the crystal axes
- Take the reciprocals
- Clear fractions
- Reduce to lowest terms and enclose in brackets ()



Intercept: 1 ∞ ∞

Reciprocal: 1 0 0

Plane: (100)

❑ Linear Density

The number of atoms per unit length for a specific crystallographic direction

$$LD = \frac{\text{number of atoms centered on direction vector}}{\text{length of direction vector}}$$

Example:

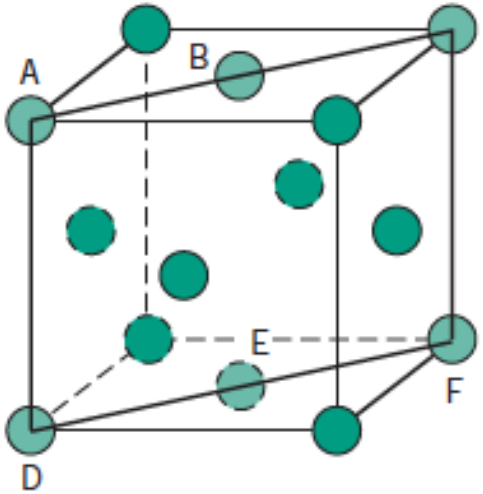
Calculate $LD_{[100]}$, $LD_{[110]}$, &$LD_{[111]}$ for FCC and BCC crystal structures

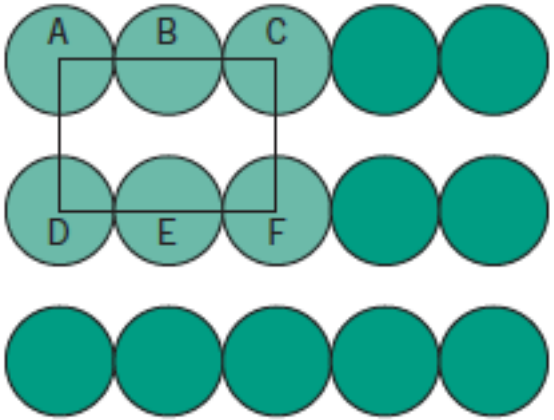
❑ Planar Density

The number of atoms per unit area for a particular crystallographic plane

$$PD = \frac{\text{number of atoms centered on a plane}}{\text{area of plane}}$$

Example: $PD_{(110)/FCC}$ for FCC crystal structure

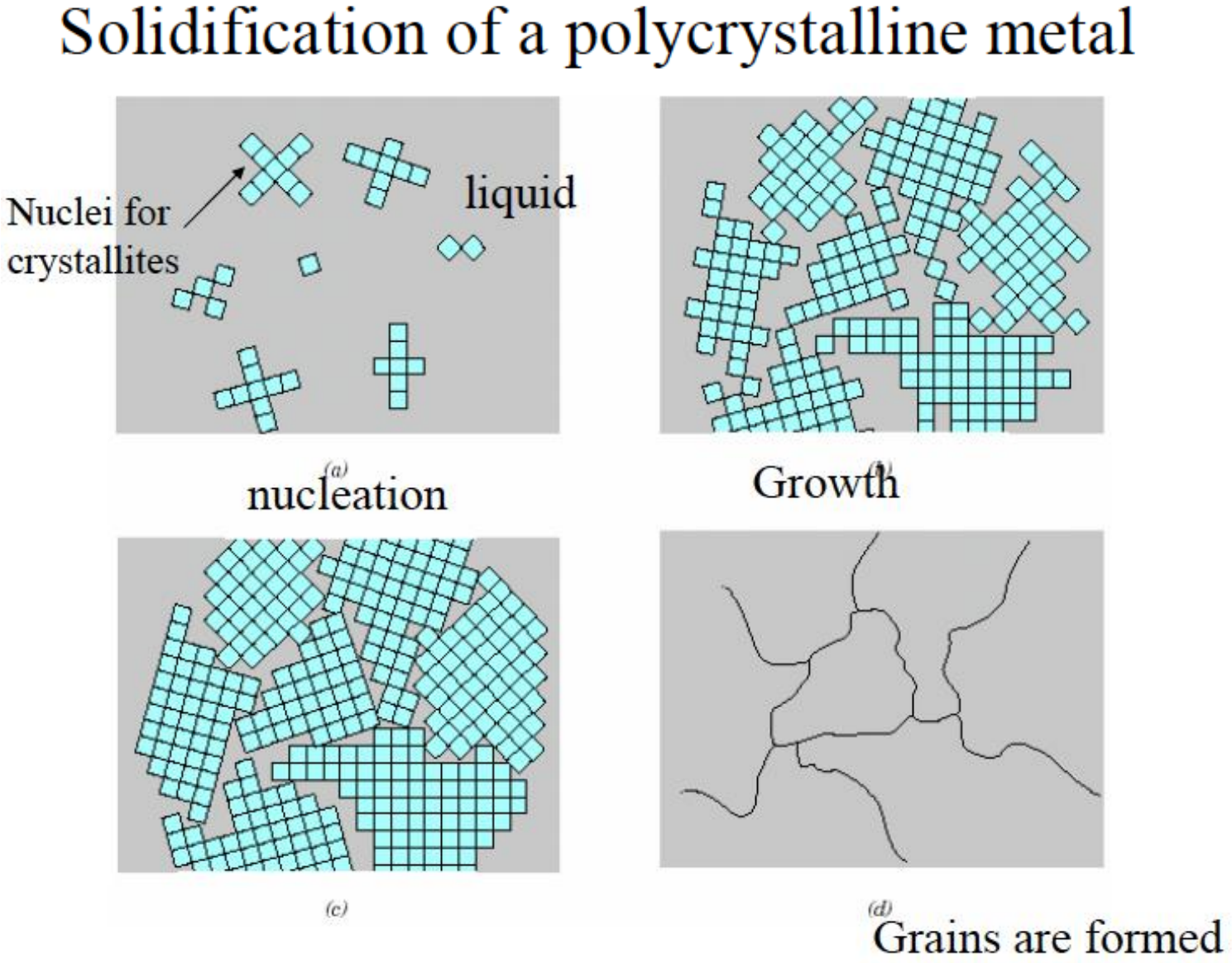




$PD_{(110)/FCC}$ = 2 atoms/(√2 a * a)

= √2 / a^2

Single crystal vs. polycrystalline materials



Main relations (Chapter 3)

$$APF = \frac{n * 4/3\,\pi R^3}{\text{Volume of unit cell}}$$

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

$$LD = \frac{\text{number of atoms centered on direction vector}}{\text{length of direction vector}}$$

$$PD = \frac{\text{number of atoms centered on a plane}}{\text{area of plane}}$$

Chapter 4
Imperfections in Solids

Types of defects

1. Point defects (0D):
   1.1) Vacancy
   1.2) Self-interstitial
   1.3) Impurities

   Substitutional and Interstitial **solid solutions**

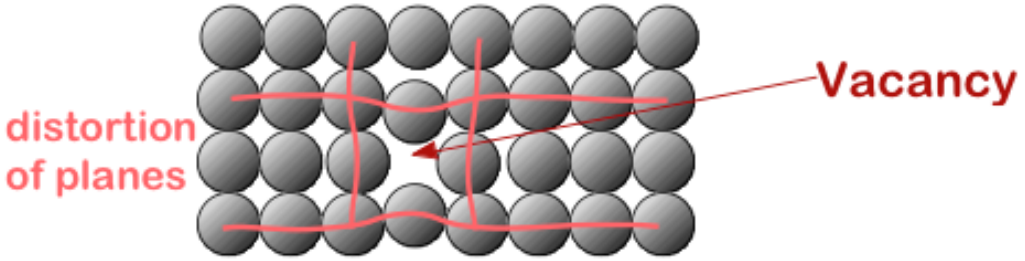
2. Line defects (1D): dislocations

3. Planar defects (2D): Grain boundaries

Defects

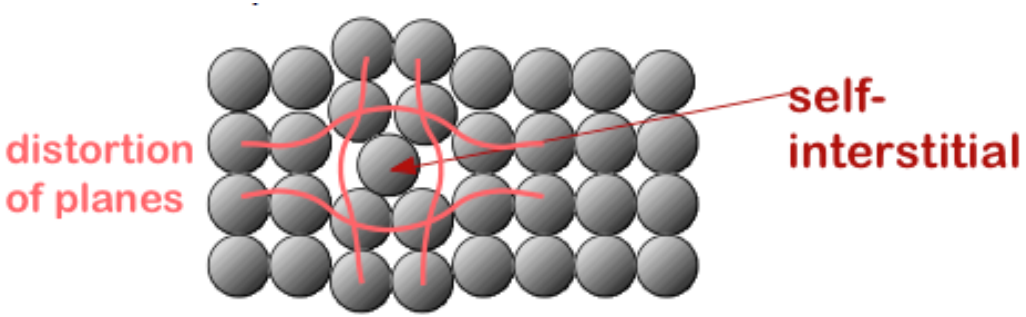
1. Point defects

1.1) Vacancy atoms



(host atoms
that occupy interstitial sites)

1.2) Self-intestinal atoms



A host atom is crowded into an interstitial site *(a space that under ordinary circumstances is not occupied)*

Equilibrium concentration of vacancies

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

N_v: Equilibrium number of vacancies

N: Total number of atomic sites

Qv: Energy required to form a vacancy

T: Temperature in Kelvin ($^oC + 273$)

K: **Boltzmann's constant**

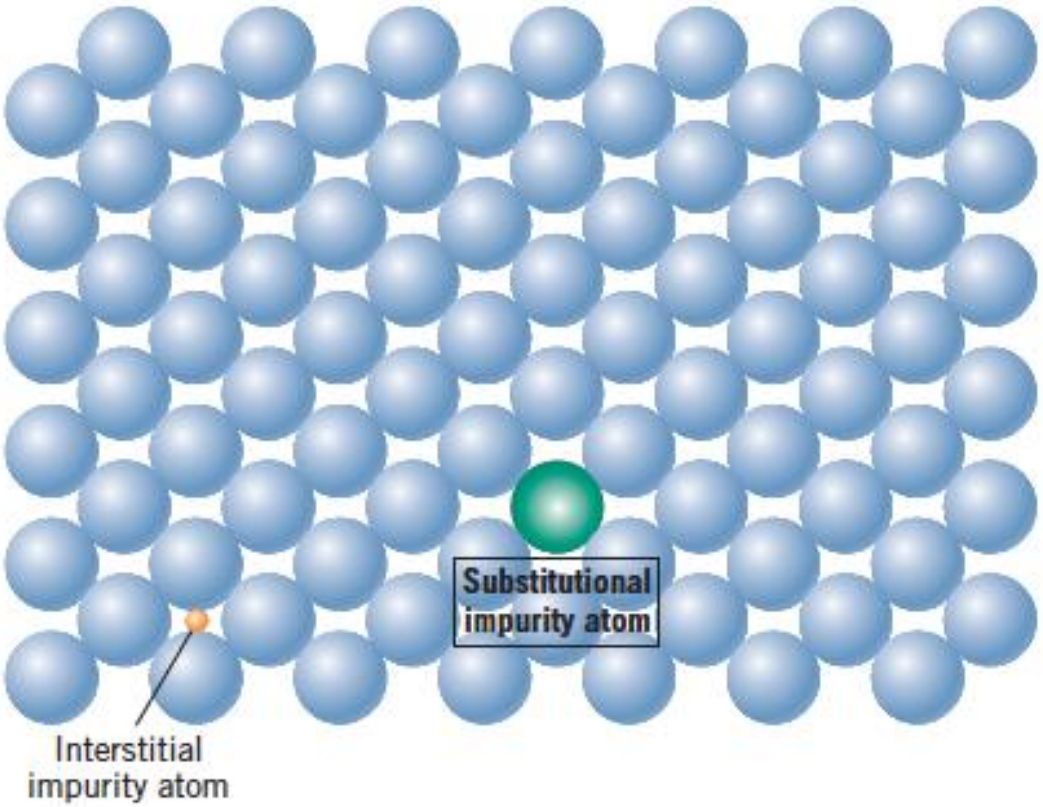
(1.38×10^{-23} J/atom K)

(8.62×10^{-5} eV/atom K)

1.3) Solid solutions: A homogenous crystalline phase that contains more than one chemical species

A. **Substitutional** solid solutions**:** The solute atoms replace or substitute for the host atoms.

B. **Interstitial** solid solutions**:** solute atoms occupy interstitial positions between the solvent atoms.



Factors that affect the complete solubility in solid solutions:

1. **Atomic size factor**: $|\Delta R\%| < 15\%$

The absolute difference in atomic radii between the two atom types is less than 15%. Otherwise, a new phase will form.

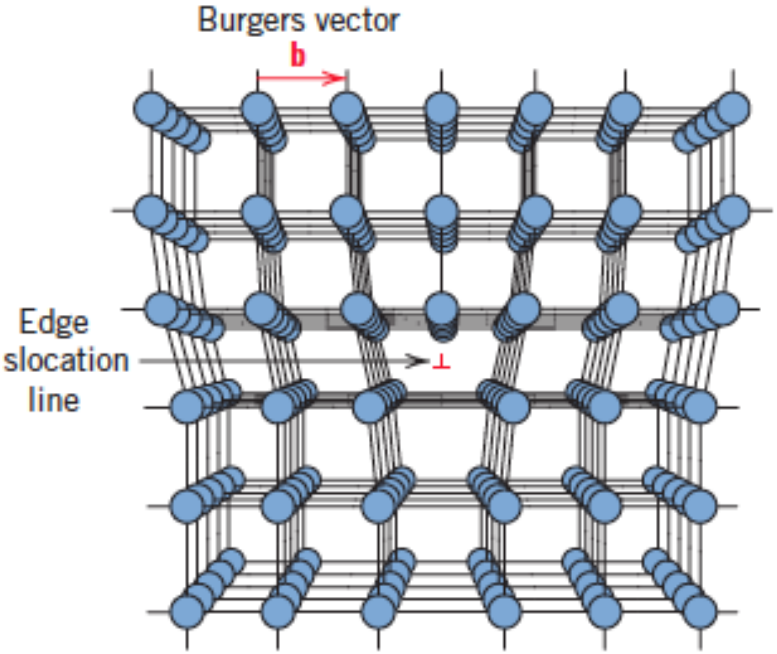
2. **Crystal structure**: The crystal structures for metals of both atom types must be the same.

3. **Electronegativity**: The electronegativities must be similar (see next slide) *(0.4 is assumed to be high)*

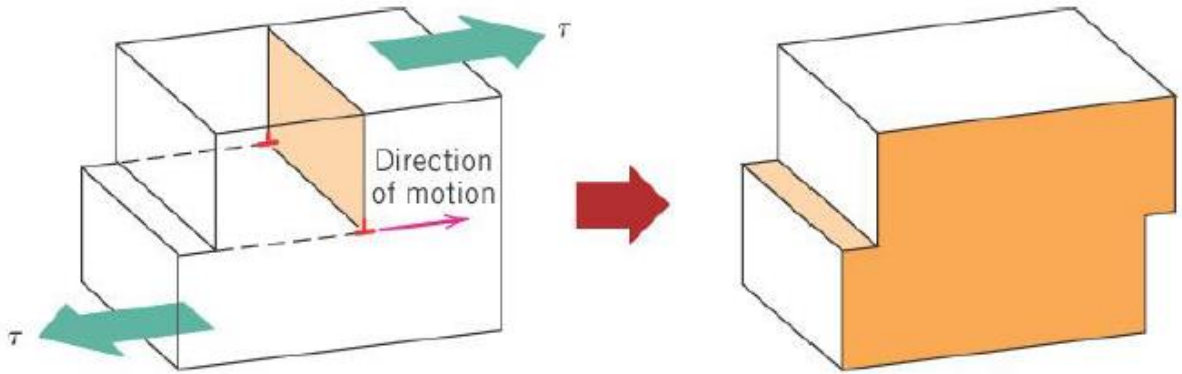
4. **Valences**: The valences should be the same, or nearly the same.

Line defects: dislocations

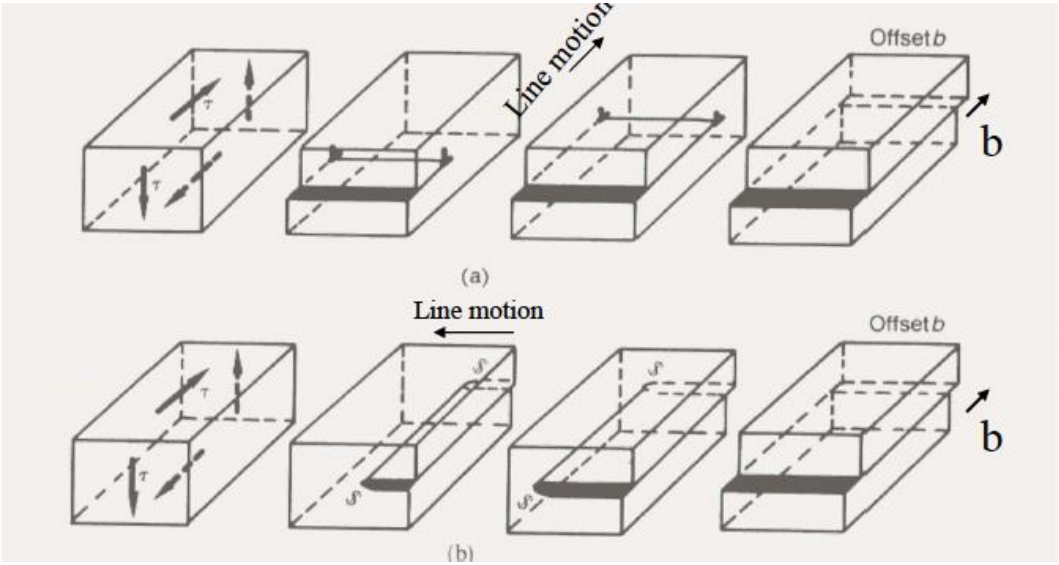
Dislocation is a linear crystalline defect around which there is atomic misalignment.



The movement of dislocations (slip) is the main reason for plastic (permanent) deformation in most metals.



Geometric properties of dislocations

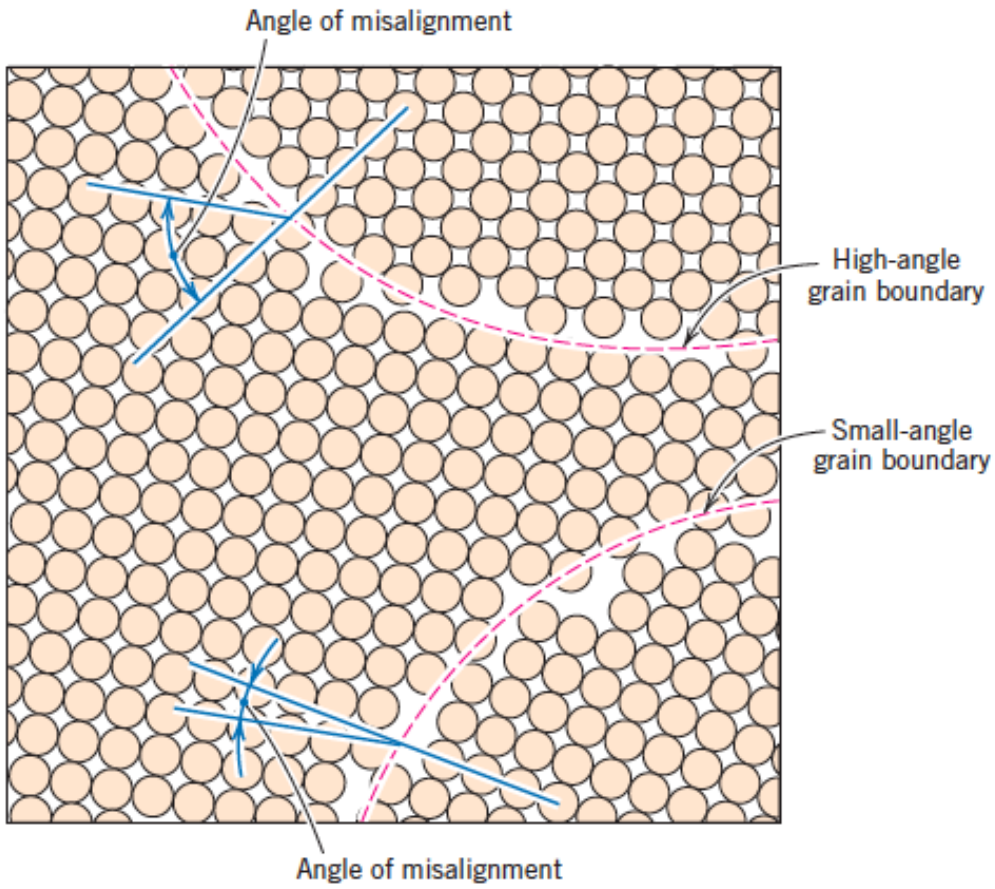


Edge dislocation

Screw dislocation

Dislocation Property	Type of dislocation	
	Edge	Screw
Relation between dislocation line (**t**) and **b**	$\perp$	$\parallel$
Slip direction	$\parallel$ to **b**	$\parallel$ to **b**
Direction of dislocation line movement relative to **b**	$\parallel$	$\perp$

❑ Planar defects: grain boundaries



Different grains have different orientations of atoms

Grain boundaries separate grains that have different lattice orientations and impede dislocation motion.

COMPOSITION

The relative content of a particular element within an alloy.

How to express the composition of an alloy?

Two descriptions

Weight %

it's based on the weight of a particular element relative to the total alloy weight

$$C_B = \frac{\text{mass of B}}{\text{total mass}} \times 100$$

Atom %

It's based on the number of moles of an element relative to the total moles of the elements in the alloy

$$C'_B = \frac{\text{\# atoms of B}}{\text{total \# atoms}} \times 100$$