Materials and Manufacturing Processes

Week 3
STRUCTURE OF MATERIALS

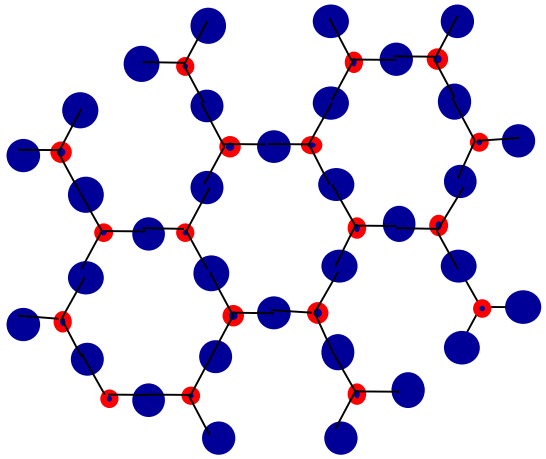
Materials Science

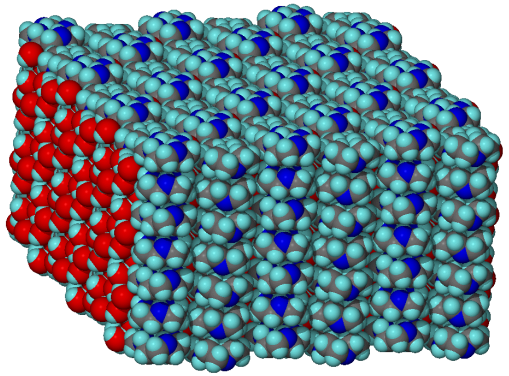
Why Study Crystal Structure of Materials?

- The properties of some materials are directly related to their crystal structures
- Significant property differences exist between **crystalline** and **noncrystalline** materials having the same composition

Crystalline and Crystal Structure

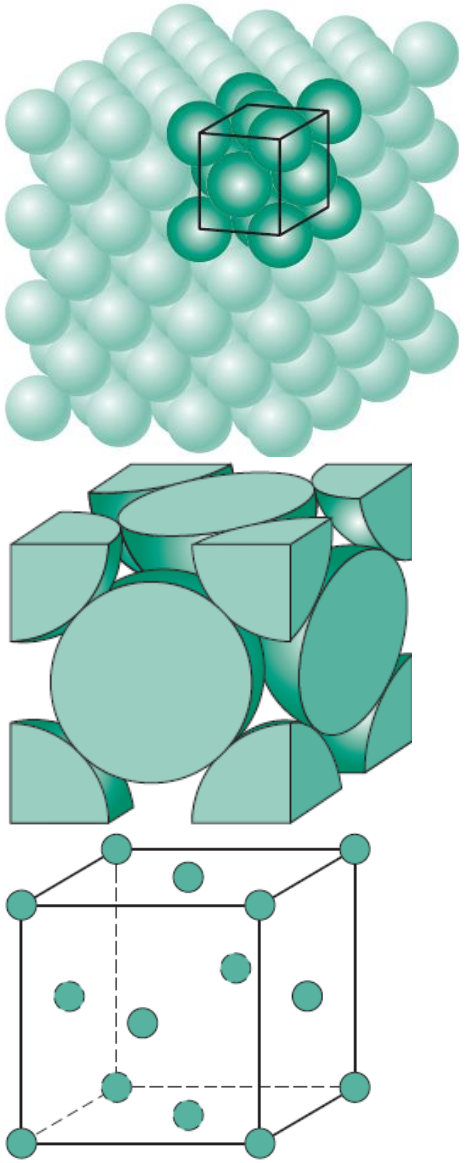
- A **crystalline** material is one in which the atoms are situated in a repeating or periodic array over large atomic distances
- All metals, many ceramics, and some polymers make crystalline structure
- Some of the properties of crystalline solids depend on the **crystal structure** of the material





Lattice

- In crystalline structures, **atoms** are considered as being solid spheres having well-defined diameters
- Atomic hard sphere model -> in which spheres representing nearest-neighbor atoms touch one another
- **Lattice** is a regularly spaced array of points that represents the structure of a crystal



Unit Cells

- **Unit Cell** is the smallest group of atom or molecules whose repetition at regular intervals in three dimensions produces the lattices of a crystal

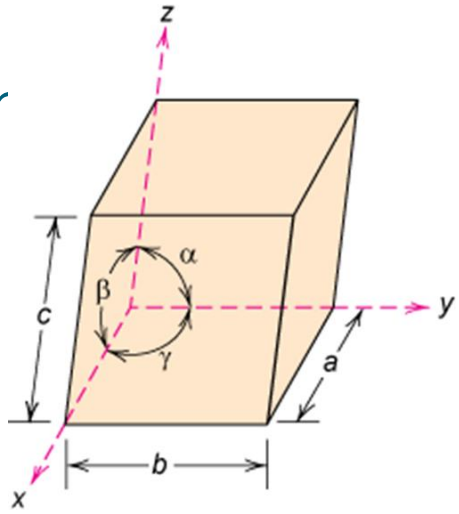
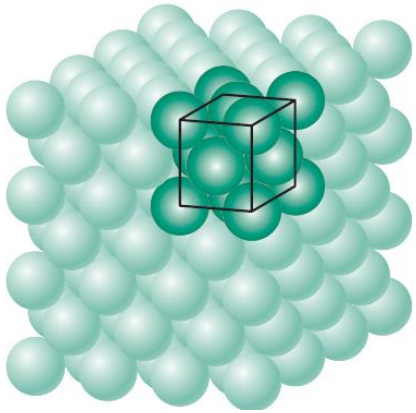


Fig. 3.4, *Callister 7e.*

- They are **parallelepipeds** or **prisms** having three sets of parallel faces

- A unit cell is chosen to represent the symmetry of the crystal structure

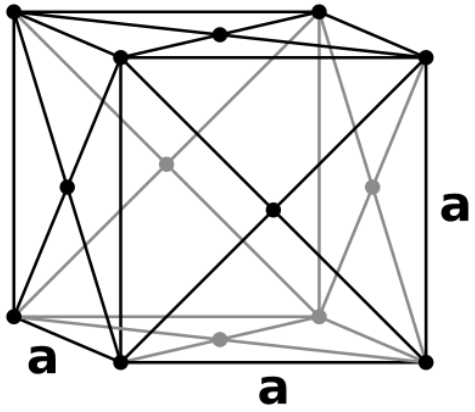


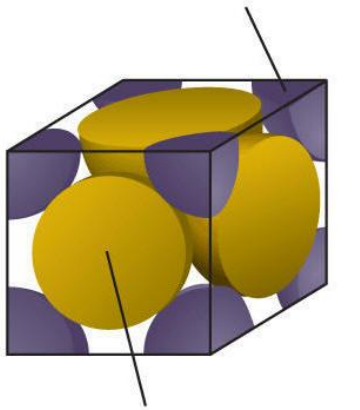
Metallic Crystal Structures

1. The Face-Centered Cubic Crystal Structure (FCC)
2. The Body-Centered Cubic Crystal Structure (BCC)
3. The Hexagonal Close-Packed Crystal Structure (HCP)

Face-Centered Cubic Structure (FCC)

- **FCC** -> a unit cell of cubic geometry, with atoms located at each of the corners and the centers of all the cube faces
- For the fcc crystal structure, each corner atom is shared among eight unit cells, whereas a face-centered atom belongs to only two
- Therefore, one-eighth of each of the eight corner atoms and one-half of each of the six face atoms, or a total of **four** whole atoms, may be assigned to a given unit cell
- copper, aluminum, silver, and gold have FCC
- The cell comprises the volume of the cube, which is generated from the centers of the corner atoms



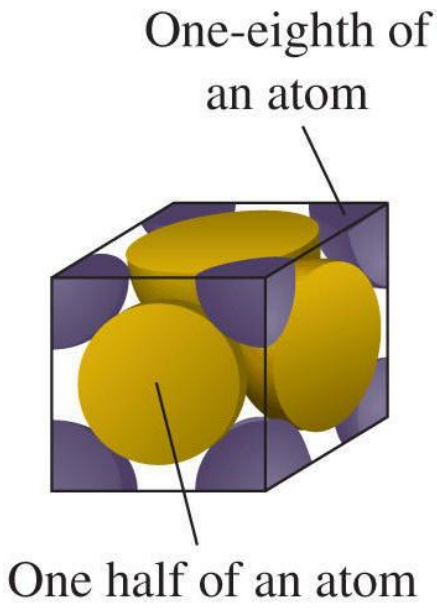


FCC - Exercise

Derive: $a = 2R\sqrt{2}$

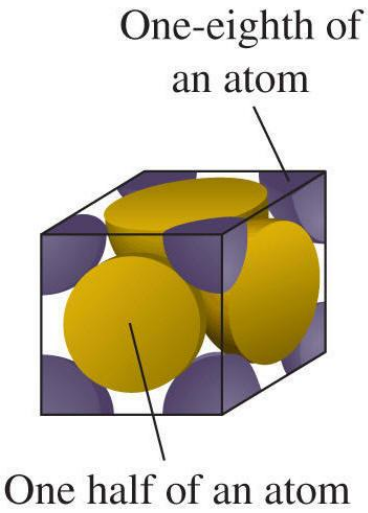
Where **a** = side length of the unit cell cube

And **R** = Radius of the atom sphere



FCC – Coordination Number and APF

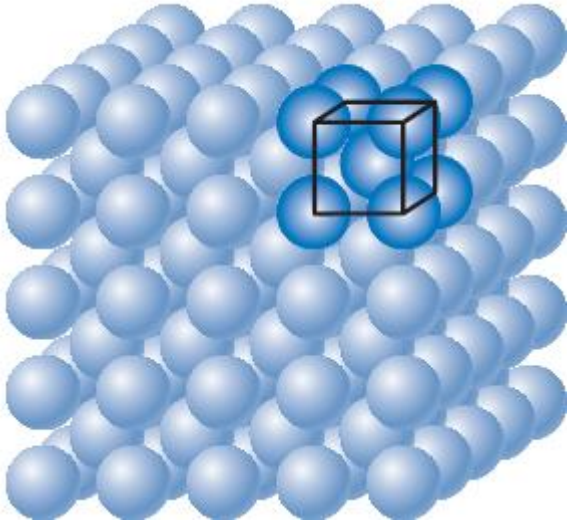
- For metals, each atom has the same number of touching atoms, which is the **coordination number**
- For **FCC**, coordination number is **12**
- The **APF** (Atomic Packing Factor) is the sum of the sphere volumes of all atoms within a unit cell divided by the unit cell volume
- For FCC, **APF** is **0.74**

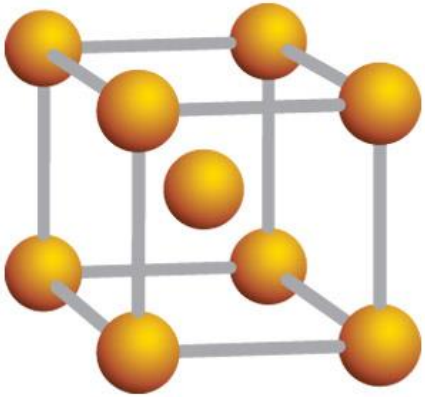


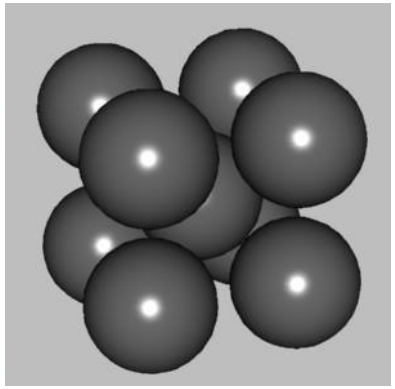
$$\text{APF} = \frac{\text{volume of atoms in a unit cell}}{\text{total unit cell volume}}$$

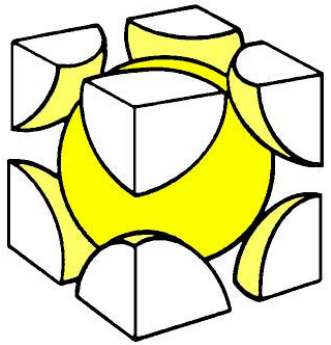
Body-Centered Cubic Structure (BCC)

- **BCC** -> a cubic unit cell with atoms located at all eight corners and a single atom at the cube center
- Center and corner atoms touch one another along cube diagonals

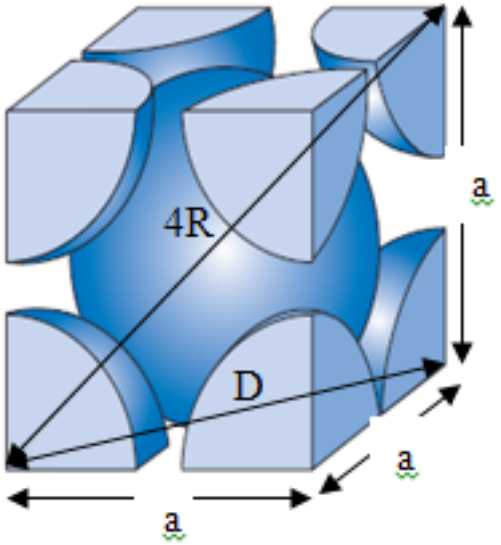








BCC - Exercise

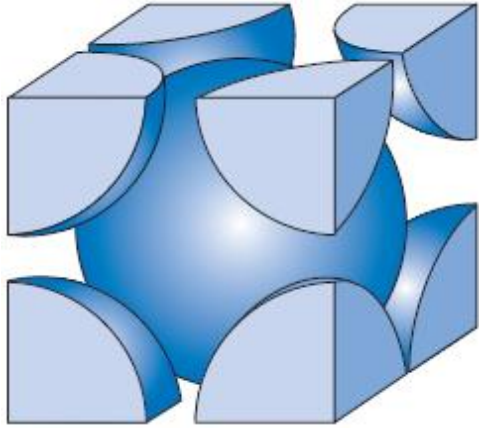


$$D^2 = a^2 + a^2 = 2a^2$$

$$(4R)^2 = D^2 + a^2 = 2a^2 + a^2 = 3a^2$$

$$a^2 = (4R)^2/3$$

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

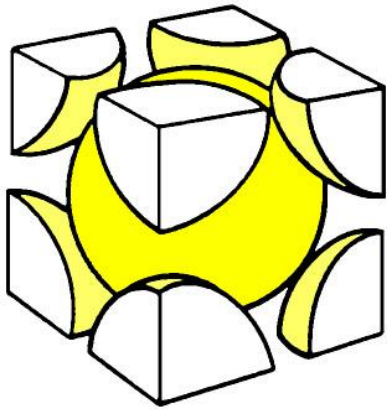


Where **a** = side length of the unit cell cube

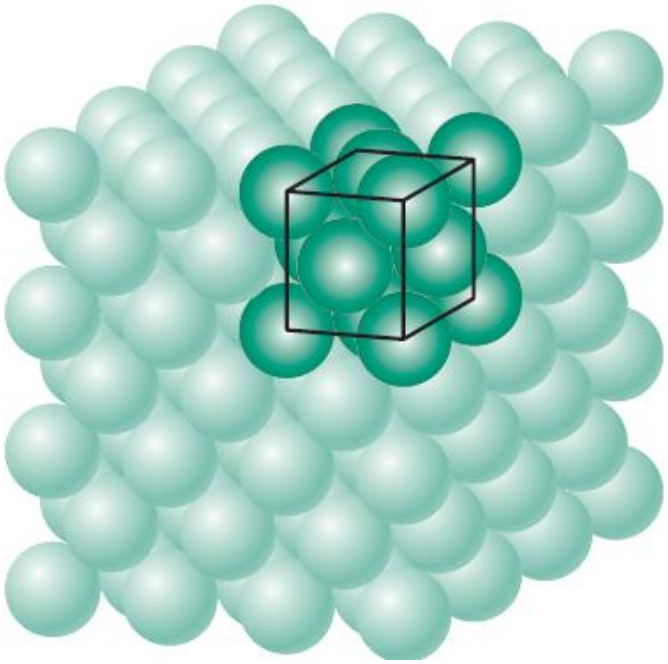
And **R** = Radius of the atom sphere

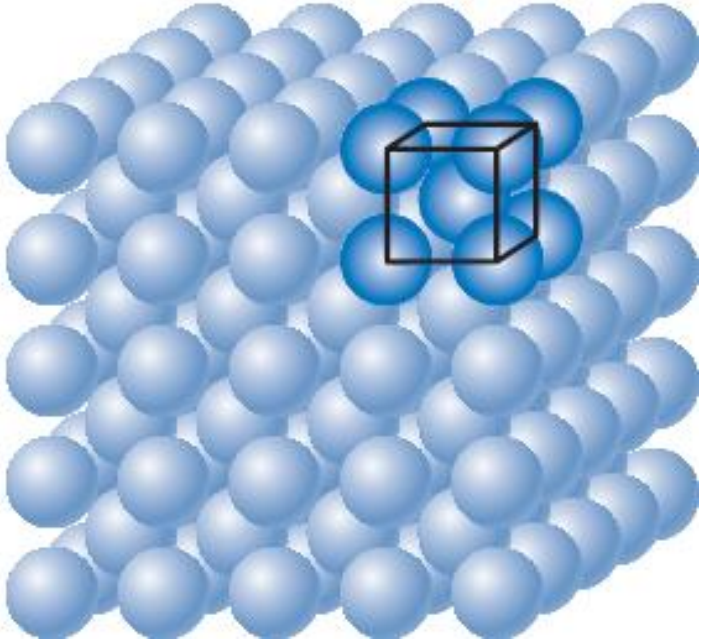
BCC

- Chromium, iron, tungsten exhibit **BCC** structure
- Two atoms are associated with each BCC unit cell
- The coordination number for the BCC is **8**
- the atomic packing factor for BCC lower—**0.68** versus **0.74** (FCC)



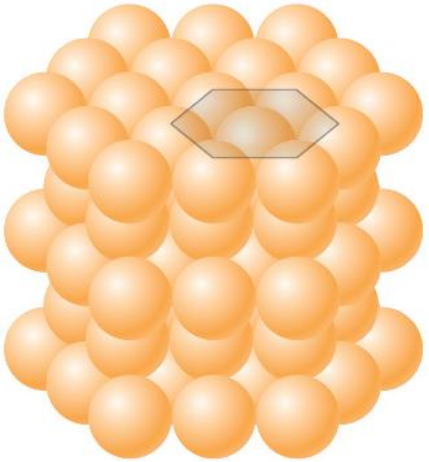
Packing Factor – FCC vs BCC

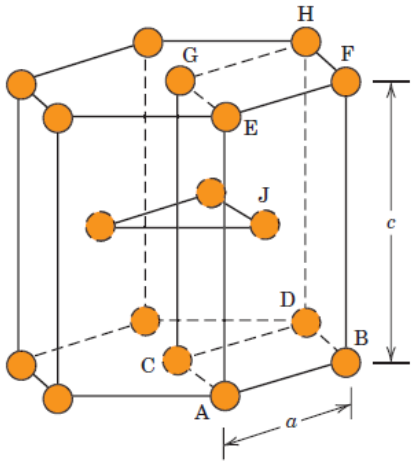




Hexagonal Close-Packed Crystal (HCP)

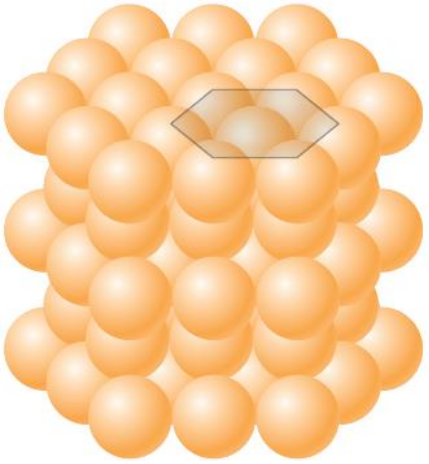
- The top and bottom faces of the unit cell consist of 6 atoms that form regular hexagons and surround a single atom in the center
- Another plane that provides 3 additional atoms to the unit cell is situated between the top and bottom planes
- The atoms in this mid-plane have as nearest neighbors atoms in both of the adjacent two planes

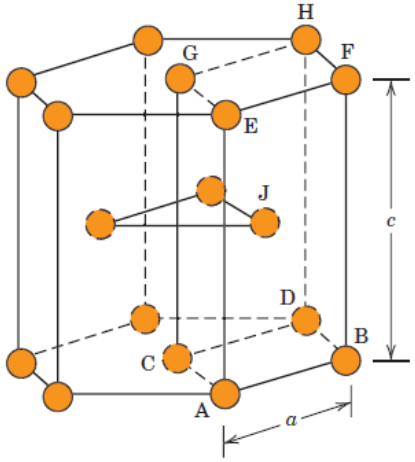




Hexagonal Close-Packed Crystal (HCP)

- The equivalent of **six atoms** is contained in each unit cell
- If *a* and *c* represent, respectively, the short and long unit cell dimensions the ***c/a*** ratio should be **1.633**
- The **coordination number** and the **APF** for the HCP are the same as for FCC: **12** and **0.74**, respectively
- The HCP metals include cadmium, magnesium, titanium, and zinc, etc





Density Computations

Density of a material can be computed from its crystalline structure,

n = *number of atoms associated with each unit cell*

A = *atomic weight*

$\boldsymbol{V_C}$ = *volume of the unit cell*

N_A = *Avogadro's number (6.023 X* 10^{23} *atoms/mol)*

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

EXAMPLE PROBLEM 3.3

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

Solution:

The crystal structure is **FCC**, **n = 4**

A_{Cu} = 63.5g/mol

$V_C = a^3 = [2R(2)^{1/2}]^3$ *(For FCC)* $= 16R^3(2)^{1/2}$; *R (atomic radius) = 0.128nm*

Using the equation:

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

EXAMPLE PROBLEM 3.3

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

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

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

- The literature value for density for Cu is **8.94g/cm³**

Crystalline and Non Crystalline Materials

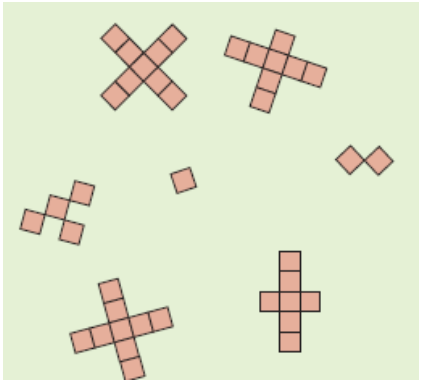
1. Single Crystal
2. Polycrystalline Materials
3. Anisotropy

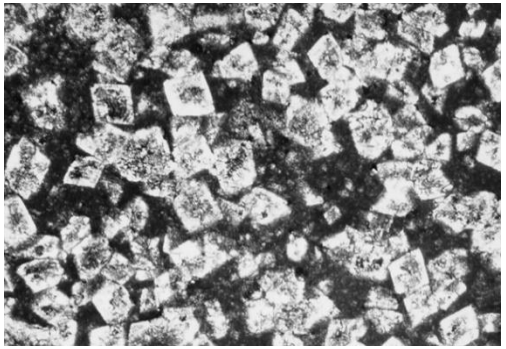
1. Single Crystal

- For a crystalline solid, when the repeated arrangement of atoms is perfect or extends throughout the specimen without ***interruption***, the result is a **single crystal.**
- If the extremities of a single crystal are permitted to grow without any external constraint, the crystal will assume a regular geometric shape having flat faces.
- Within the past few years, single crystals have become extremely important in many of our modern technologies.

2. Polycrystalline Materials

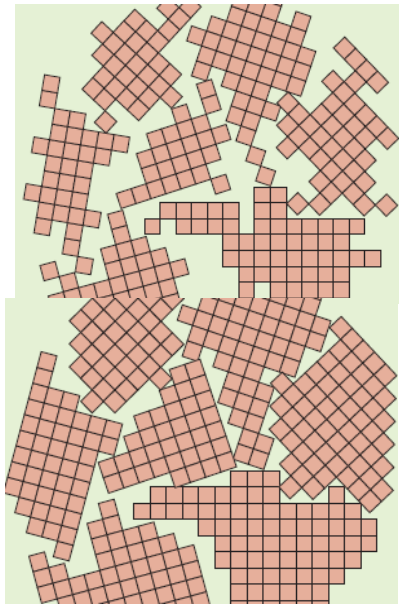
- Most crystalline solids are composed of a collection of many small crystals or **grains;** such materials are termed **polycrystalline**
- Initially, small crystals or nuclei form at various positions. These have random crystallographic orientations

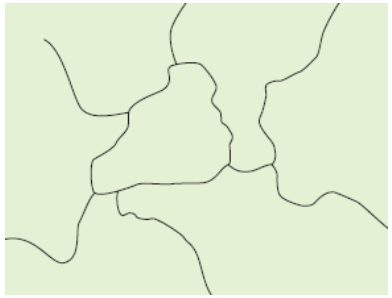




2. Polycrystalline Materials

- Growth of the crystallites; the obstruction of some grains that are adjacent to one another
- Upon completion of solidification, grains having irregular shapes have formed
- There exists some atomic mismatch within the region where two grains meet; this area, called a **grain boundary**
- The grain structure as it would appear under the microscope; dark lines are the grain boundaries





3. Anisotropy

- The physical properties of single crystals of some substances depend on the crystallographic direction in which measurements are taken
- This directionality of properties is termed **anisotropy.**

- The extent and magnitude of anisotropic effects in crystalline materials are functions of the symmetry of the crystal structure

3. Anisotropy

- For many polycrystalline materials, the crystallographic orientations of the individual grains are totally random.
- Under these circumstances each grain may be thought of anisotropic region but a specimen composed of the grain aggregate behaves isotropically.
- Sometimes the grains in polycrystalline materials have a preferential crystallographic orientation, in which case the material is said to have a '**texture**'.