EGN 3365
Review on Bonding & Crystal Structures

FLORIDA INTERNATIONAL UNIVERSITY

Expectations on Chapter 1

❑Chapter 1

- Understand materials can be classified in different ways by composition, property, application, or other aspects.
- Be able to enumerate major categories of materials in terms of composition: i.e., metals, ceramics, polymer, and composite and describe briefly the characteristics of each type of materials
- Be able to name the major factors or perspectives when dealing with engineering materials: i.e., composition, processing, structure, property (and performance) and understand that those factors often have close interdependence/relationships among them

Expectations on Chapter 2

❑Chapter 2

- Understand basic concepts including their units such as atomic number, atomic weight (or mass), number of protons, number of electrons, isotopes. Be able to correctly identify those if given sufficient information (e.g., a periodic table)
- Be able to understand concept of valence electrons and its impact on materials chemical and other properties
- Be able to enumerate three major types of primary bonding, i.e., ionic bond, covalent bond, and metallic bond and describe briefly their major characteristics and understand the relationship between electronegativity and the type of primary bond
- Understand that there exist secondary bonds between molecules such as van der Waals bond and hydrogen bond. Understand hydrogen bond is strongest among secondary bonds occurring between molecules containing both hydrogen and highly electronegative atoms of oxygen, fluorine, or nitrogen

Expectations on Chapter 3 (1)

❑Chapter 3

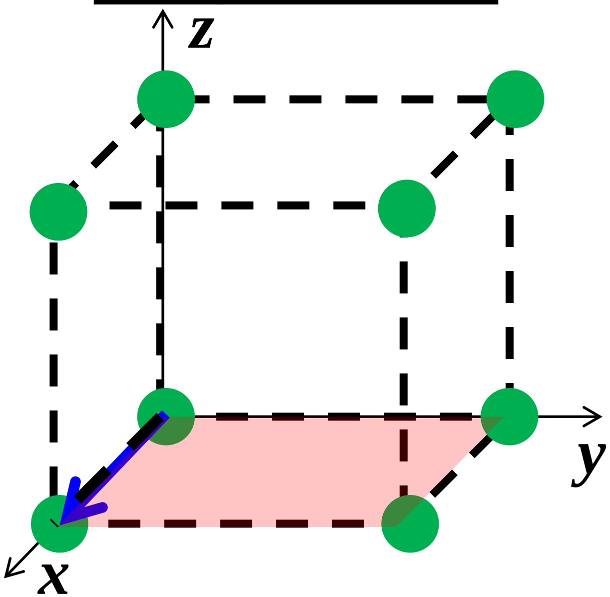
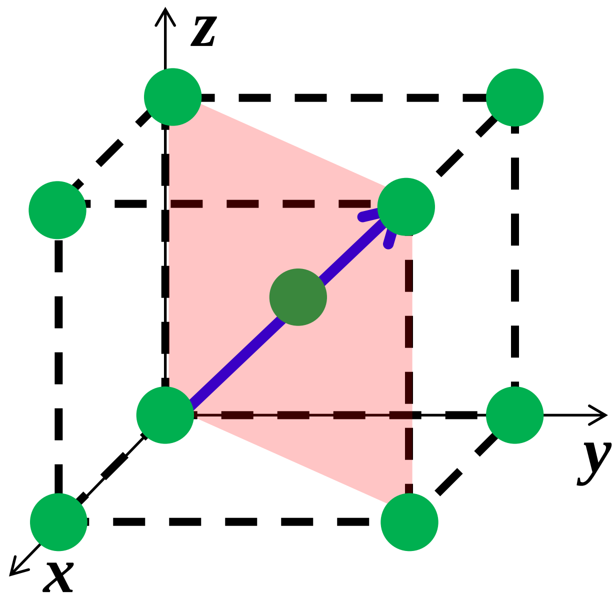
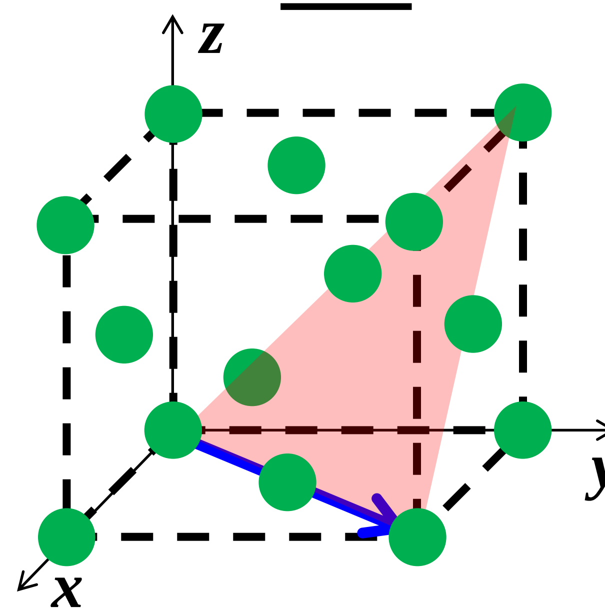
- Understand the difference between crystalline and non-crystalline (amorphous materials) and the difference between single crystal and polycrystalline materials
- Understand the concepts of lattice, unit cell, coordination number, nearest neighbor for crystals
- Understand different crystal systems
- For simple cubic, body centered cubic (BCC), and face centered cubic (FCC) structures and other related structures given sufficient information, be able to draw the unit cell structures and obtain coordinates and indices for points, directions, and crystal planes and vice versa or draw those if given coordinates/indices. Also be able to derive
  - Coordination number
  - The number of atoms per unit cell
  - The relationship between atom size (radius) and lattice parameter (unit cell edge length) for simple geometry
  - Atom packing factor (APF) in 3D
  - Theoretical density if given atom radius or atom radius if given density

Expectations on Chapter 3 (1)

❑ Chapter 3 (continued)

- Understand the concepts of closed packed direction, close packed plane, and close-packed structures of HCP and FCC
- Understand concepts of polymorphism and anisotropy
- Understand X-ray diffraction technique could be used to determine crystal structures

Close Packed Direction & Planes of Highest Planar Density in Cubic Crystals

Simple Cubic	BCC	FCC
		

Close Packed Direction

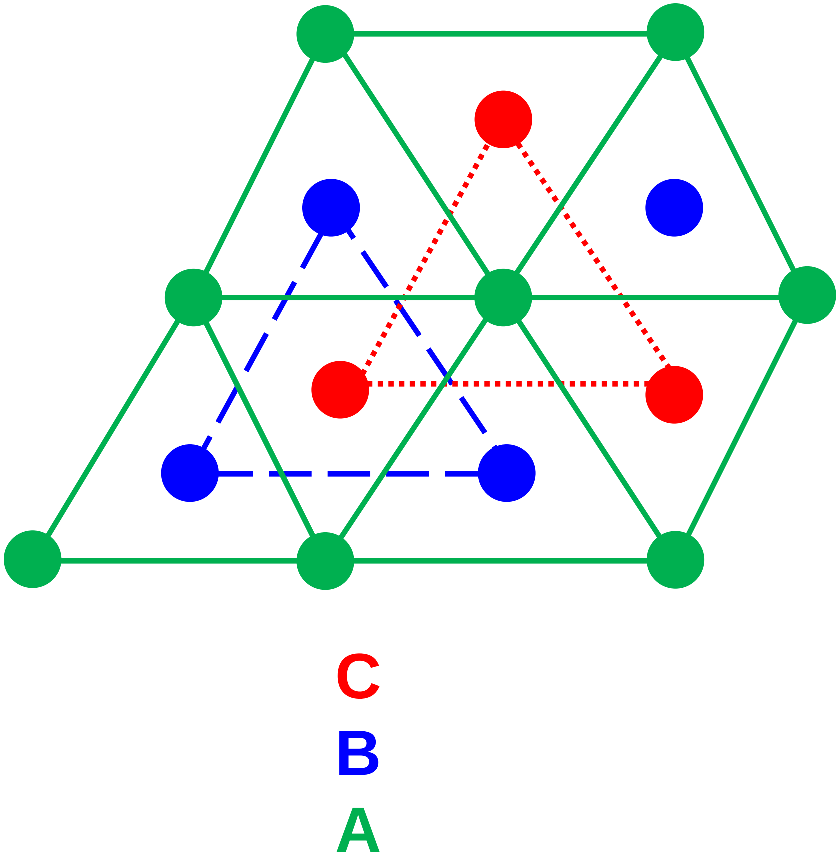
Simple Cubic	BCC	FCC
<100>	<111>	<110>

Plane with Highest Planar Density

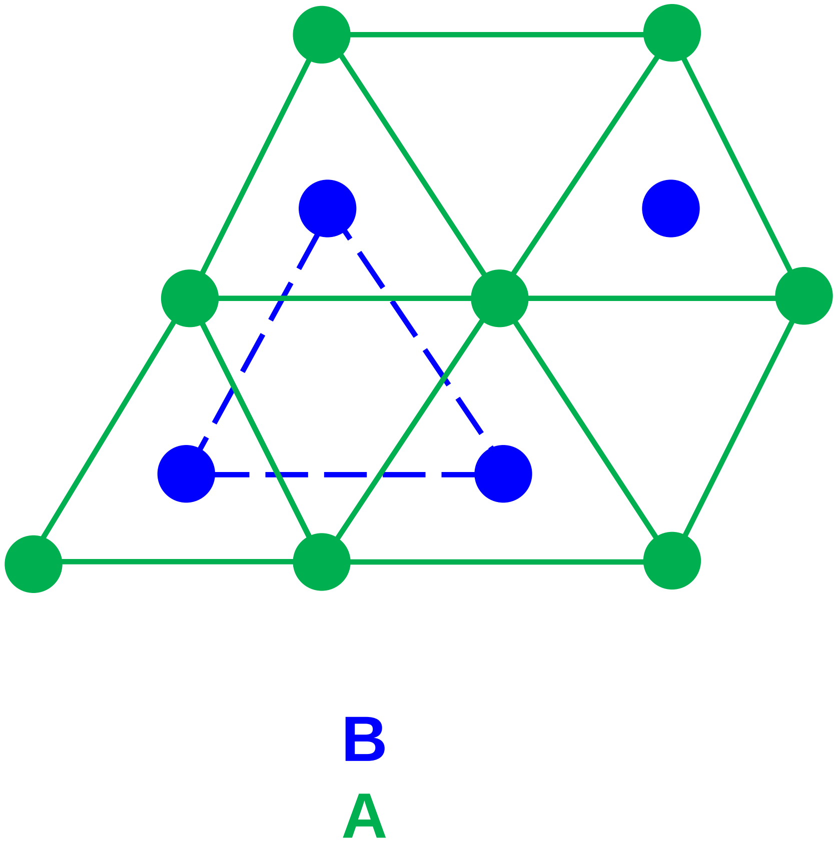
Simple Cubic	BCC	FCC
{100}	{110}	{111}

Close Packed Structures

FCC

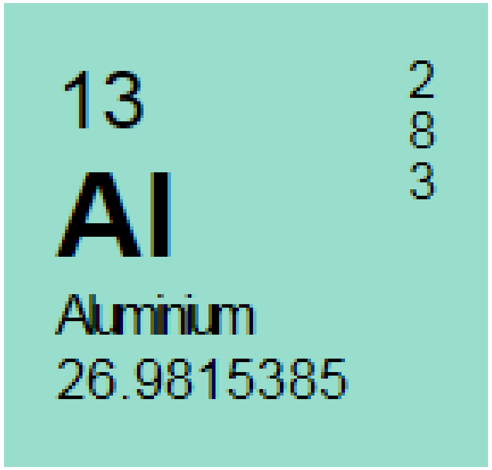


HCP



Class Exercise – Periodic Table

- **Given information on right from periodic table for aluminum,**



- What is the atomic number Z

13

- What is the number of proton in Al nucleus

13

- What is the atomic weight A and the unit for atomic weight A

26.98 g/mol

- On average, one gram of Al will contain how many Al atoms?

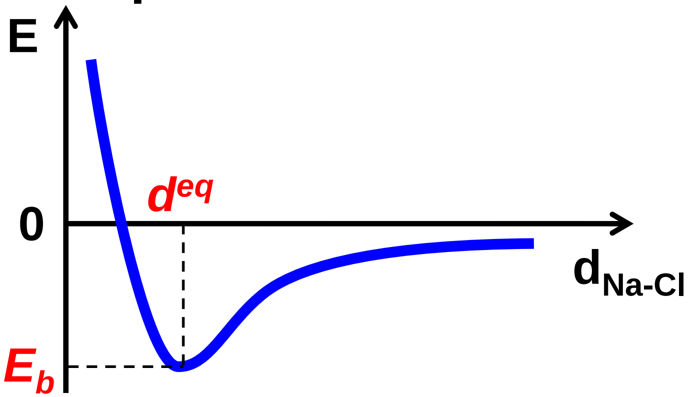
$$\frac{1}{A} \cdot N_A = \frac{1g}{26.98g/mol} \cdot 6.02 \times 10^{23}/mol = 2.23 \times 10^{22}$$

- What is the averaged (over naturally occurring isotope) mass (weight) for one aluminum atom?

$$\frac{A}{N_A} = \frac{26.98g/mol}{6.02 \times 10^{23}/mol} = 4.48 \times 10^{-23} g$$

Class Exercise - Bonds

- **Roughly plot the change of <u>total</u> potential energy with respect to interatomic distance *d* between Na and Cl atoms in NaCl and explain the physical meaning of the features in the plot**
  - Zero energy when atoms separated far away
  - Very high energy when atoms pushed very close
  - Bonding energy E_b
  - Equilibrium distance d^{eq}



- **Given the following electronegativity numbers**
  - χ (Na)=0.9; χ (F)=4.0; χ (Si)=1.8; χ (C)=2.5; χ (Mg)=1.2;

Determine the predominant primary bond type in the follow materials

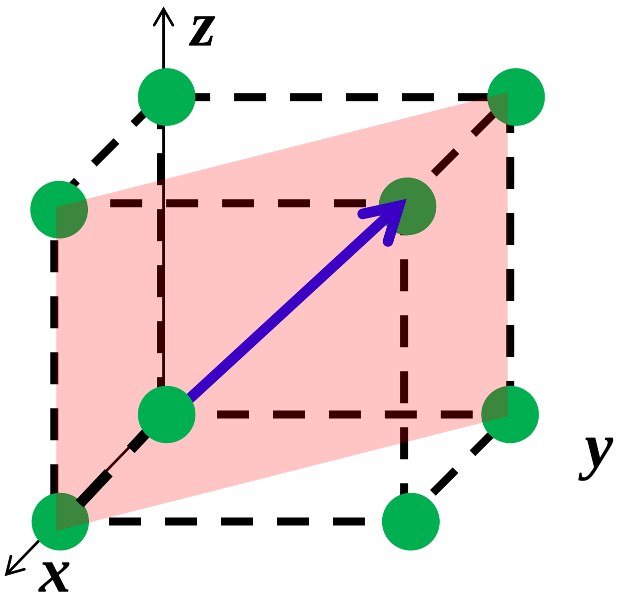
- Sodium fluoride (NaF) — Ionic bond
- Silicon carbide (SiC) — Covalent bond
- Pure magnesium (Mg) — Metallic bond

Class Exercise – Crystal Structure (1)

For a pure metal with simple cubic structure

- ❑**Draw the lattice structures and label the axis**
- ❑**Give coordination number (the number of nearest neighbors) for an atom in the structure**
- ❑**Give the average number of atoms in a unit cell for the simple cubic structure and explain why**
- ❑**Given atoms radius of R, calculate**
  - The distances between center of one atom to its nearest neighbors and to its 2nd nearest neighbors, respectively
  - Label [111] direction and (110) plane
  - Theoretical density if given atom mass of A (in unit of g/mol) and Avagadro's constant N_A
  - *Atom linear density along [111] direction and area density for (110) plane (**NOT requirement for exam**)*

Class Exercise – Crystal Structure (2)



- **Number of nearest neighbor = 6**
- **Number of atoms in unit cell: 8x(1/8)=1**
- **Distance to nearest neighbor: *2R***
- **Distance to 2nd nearest neighbor:** $2\sqrt{2}R$
- **Atoms linear density along [100] direction:**

$$LD_{[100]} = \frac{1}{2R}$$

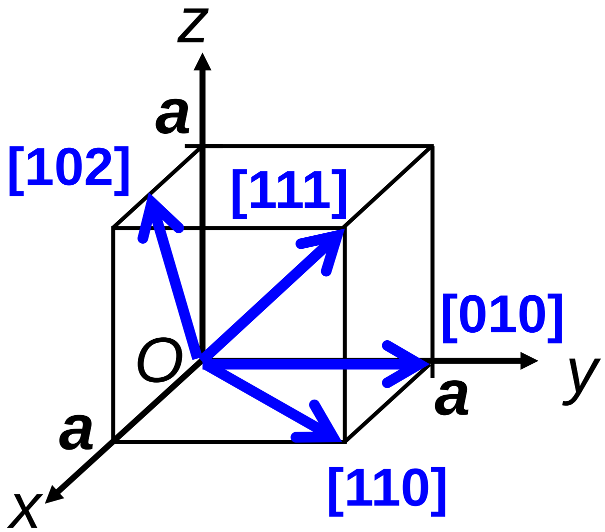
- **Atoms planar density along (100) plane:** $PD_{(110)} = \frac{1}{4R^2}$

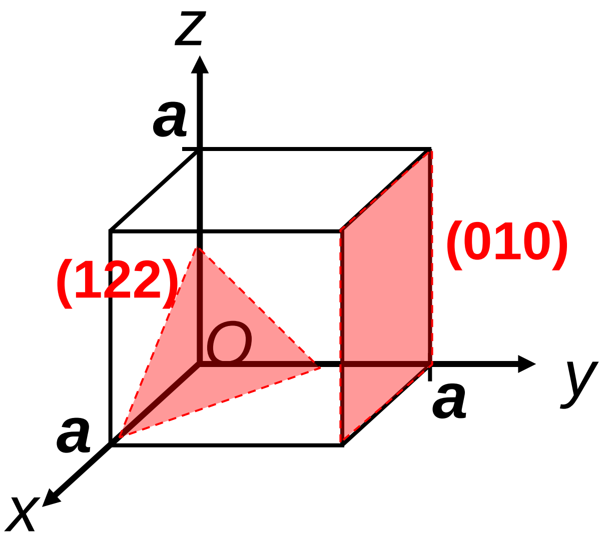
- **Theoretical density:**

$$\rho_{theo} = \frac{1\frac{A}{N_A}}{(2R)^3} = \frac{A}{8R^3 N_A}$$

Class Exercise – Direction and Plane Indices

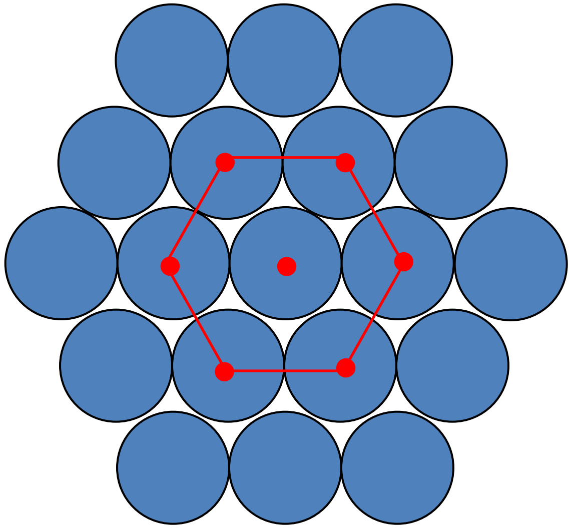
- **Based on the coordinate system given, draw [010], [110], [111], and [102] directions**
- **Based on the coordinate system given, draw (010), (122) and planes**



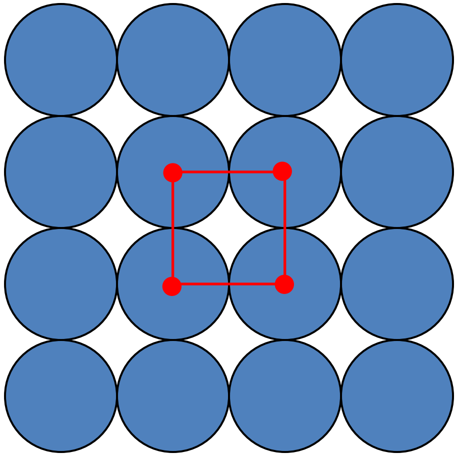


Class Exercise – Crystal Structure (3)

Using the concepts for lattice and unit cell, for <u>2D</u> structure (of the same atoms) given below, please try to draw the <u>2D</u> unit cell and determine the coordination number (CN) and number of atoms per unit cell (n)



CN (# of nearest neighbor) = 6
Number of atoms per unit cell = 1+6x1/3 = 3



CN (# of nearest neighbor) = 4
Number of atoms per unit cell = 4x1/4 = 1