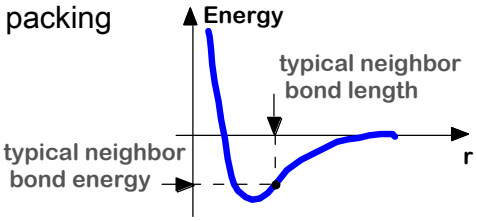
Outline:

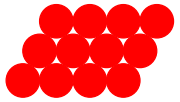
- Crystalline versus amorphous structures
- Crystal structure
  - Unit cell
  - Coordination number
  - Atomic packing factor
- Crystal systems

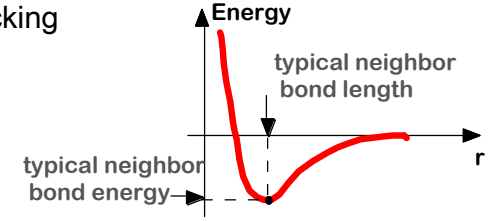
ENERGY AND PACKING

- Non dense, random packing



- Dense, regular packing

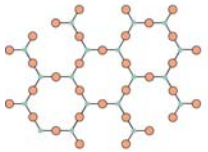




Dense, regular-packed structures tend to have lower energy.

MATERIALS AND PACKING

Crystalline materials...
- atoms pack in periodic, 3D arrays
- typical of: -metals
  -many ceramics
  -some polymers

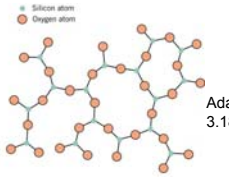


Adapted from Fig. 3.23(a), *Callister 8e.*

crystalline SiO_2

Noncrystalline materials...
- atoms have no periodic packing
- occurs for: -complex structures
  -rapid cooling

…….... = Noncrystalline



Adapted from Fig. 3.18(b), *Callister 6e.*

noncrystalline SiO_2

Atoms can be arranged either in a regular, periodic array (i.e., long-range order) or completely disordered (amorphous).

Crystal Structure

- Motivation: Many of the properties of materials (*especially mechanical*) are determined by the arrangement of the constituent atoms.

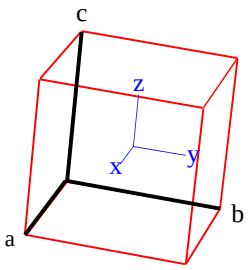
  This arrangement is called the material's crystal structure.

- An important distinction…
  - Atomic structure relates to the number of protons and neutrons in the nucleus of an atom, as well as the number and probability distributions of the constituent electrons.
  - On the other hand, crystal structure pertains to the arrangement of atoms in the crystalline solid material.

Crystal Structure

- We need a way to specify crystallographic directions and planes.
- Let's start with the hard sphere model (in which nearest neighbor atoms "touch" each other)…

To illustrate the concept of crystal structure and lattice systems, we first identify a coordinate system (x, y, z):

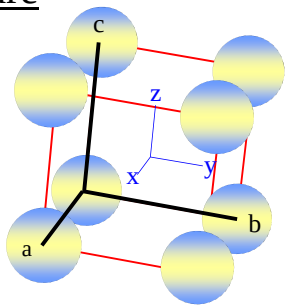


We can't specify directions or planes without knowing what the reference system is.

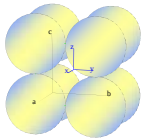
Crystal Structure

Now place an atom at each corner…

This represents the "hard sphere" model of a …….. crystal system



- Atoms "touch" along the crystal axes
- These directions are referred to as "close-packed" in the simple cubic system



not many examples of simple cubic systems in nature, except for Po

The above diagram represents a simple cubic ……..

What is Unit Cell?

- A unit cell is the smallest entity that exhibits the chemical and …… properties of the material.

  – *Unit cells are the most elementary arrangement of atoms which can generate the entire crystal upon application of suitable translation, rotation, mirror, or inversion operations.*

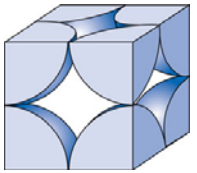
Definition:

the length of each unit cell axis is called a ……..

– *In cubic systems, all three orthogonal lattice parameters are equal*

– Lattice parameters are typically on the order of a few Angstroms (or a few tenths of a nanometer)

Simple Cubic Unit Cell



How many atoms does the simple cubic unit cell contain?

You should be able to convince yourself that a simple cubic structure contains … atom/unit cell.

(Remember, a part of each atom is shared by another unit cell!)

- The number of atoms/unit cell is an important quantity and determines many physical properties.
- In general, the number of atoms/unit cell, N, is given by

$$N = N_i + \frac{N_f}{2} + \frac{N_c}{8}$$

Where: N_i = # interior atoms,
N_f = # face atoms,
N_c = # corner atoms

Simple Cubic Unit Cell

- volume of the unit cell = a^3
  - where a is the lattice parameter
- coordination # = 6
  - for simple cubic structures

✓CN is the number of nearest-neighbor atoms

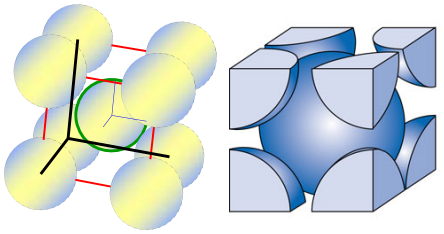
✓ Coordination number is important in determining the structure of crystalline materials.

✓ Large atoms tend to have large CN, small atoms usually have small CN

it's easier to surround a big atom with lots of atoms than a smaller one.

Body Centered Cubic Unit Cell

Now, suppose we add another atom at the **center** of the cube



We no longer have a simple cubic structure but instead, a …… ……..….. (BCC) structure

Examples of BCC systems: Cr, W, Mo, Ta, Fe (αFe stable below 912°C)

Notice that in the BCC structure, atoms touch along the body ……. These are the close-packed directions in the body-centered cubic structure.

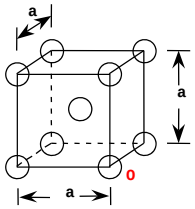
BCC unit cells have a CN = ……

Atomic Packing Factor

$$\text{Atomic Packing Factor (APF or APE)} = \frac{\text{total "sphere" volume}}{\text{total cell volume}}$$

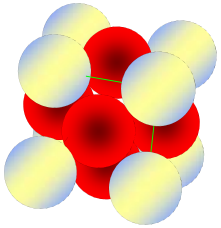
"total sphere volume" is just the volume per atomic "sphere" multiplied by the number of atoms in the unit cell

Example: Calculate the APF for a BCC unit cell:



Face Centered Cubic Unit Cell

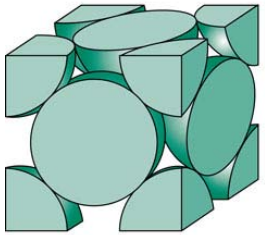
Now suppose we place equivalent atoms at the corners of the unit cell, AND in the center of each face:



This is a …… (FCC) crystal structure

- Examples of FCC metals: Cu, Ni, Au, Ag, Fe *(γFe stable above 912°C)*
- Close-packed directions in FCC metals are along face diagonals

Face Centered Cubic Unit Cell



• Q: How many atoms per unit cell in the FCC structure?

$$\text{recall, } N = N_i + \frac{N_f}{2} + \frac{N_c}{8}$$

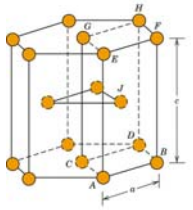
• FCC unit cells have a CN = 12 and an APF = 0.75

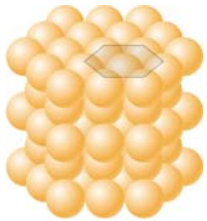
– *maximum packing efficiency for monosized spheres*

Hexagonal Unit Cell

- There are other ways in which atoms can be arranged to form unit cells:
  - For example…

This represents an HCP (.....…… ……) structure





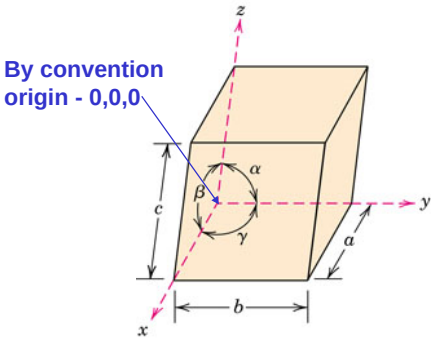
➢ Examples of HCP systems ***(Mg, Co, Ti, Zn, Zr, RE)***

➢The HCP unit cell consists of 6 atoms forming the corners of a hexagon in the basal planes + 1 atom in the center. In addition, there are 3 interior atoms midway between basal planes along the c-axis.

atoms/unit cell = (1/6)*12 (corner atoms) + (1/2)*2 (center face atoms) + 3 (interior atoms) = …….

➢ Coordination # = ……

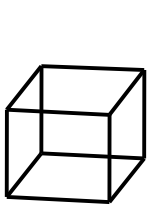
General convention for unit cell axis and angle notation:



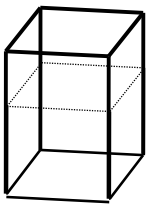
In total, there are 7 distinct and unique crystal systems:

cubic represents only one of the 7

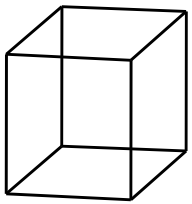
Crystal Systems



Cubic
a=b=c
α=β=γ=90

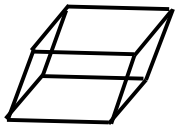


Tetragonal
a=b≠c
α=β=γ=90



Orthorhombic
a≠b≠c
α=β=γ=90

Crystal Systems

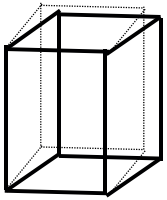


Rhombohedral

a=b=c

α=β=γ≠ 90

"Pushed over" cube



Hexagonal

a=b≠c

α=β=90 γ=120

"Squished" tetragonal

Monoclinic
a≠b≠c
α=γ = 90, β≠90

"Pushed over" orthorhombic (in one direction)

Triclinic
a≠b≠c
α≠β≠γ ≠ 90

"Pushed over" orthorhombic (in two directions)

Crystal Systems

Note that these 7 crystal systems do not account for all the possible lattice types

for example, the cubic system contains SC, FCC, and BCC as subsets

Crystal System	Axial Relationships	Interaxial Angles	Unit Cell Geometry
Cubic	$a = b = c$	$\alpha = \beta = \gamma = 90°$	
Hexagonal	$a = b \neq c$	$\alpha = \beta = 90°, \gamma = 120°$	
Tetragonal	$a = b \neq c$	$\alpha = \beta = \gamma = 90°$	
Rhombohedral	$a = b = c$	$\alpha = \beta = \gamma \neq 90°$	
Orthorhombic	$a \neq b \neq c$	$\alpha = \beta = \gamma = 90°$	
Monoclinic	$a \neq b \neq c$	$\alpha = \gamma = 90° \neq \beta$	
Triclinic	$a \neq b \neq c$	$\alpha \neq \beta \neq \gamma \neq 90°$	

Crystal Systems

There are 14 unique lattice types from this framework of 7 crystal systems (called Bravais lattices):

Crystal system	Types of possible lattice arrangements
Cubic	SC, BCC, FCC
Hexagonal	HCP
Tetragonal	Simple, body-centered
Orthorhombic	Simple, base-centered, BC, FC
Rhombohedral	Simple
Monoclin	Simple, base-centered
Triclinic	Simple

We will mainly be concerned with cubic and hexagonal systems in this class. But you need to realize that many other types of symmetries exist!

Next time:

Crystallographic Directions and Planes