Lecture 5

Monday, April 07, 2008
10:39 AM

http://courses.washington.edu/mse170/index.shtml

References Used:

1. B D Cullity, **Elements of X-ray Diffraction, 2nd Edition**, *Addison Wesley*, 1978.

Course Notes

1. There is a new whatever you want box -- note that it is the black leather box in the back.

2. Possible part time position at CASE Forensics
   - 10-20 hours per week
   - $10-15 per hour
   - If you are interested -- send me an email with your resume

Review

- We talked about crystallinity -- how a crystal is defined by long range order
- We talked about point lattices -- how to simplify understanding of atomic organization in a crystal we can reduce each atom to a single point
- We talked about a unit cell
  - We talked about how a unit cell is described by 3 vectors: **a, b, c**
  - Those vectors can be described by the lattice constants or lattice parameters which are three lengths a, b, c and three angles α, β, γ
- We noted that there are 7 crystal systems and 14 Bravais Lattices
- These 14 can be used to describe all possible unit cells

Add one thing:

The number of lattice points per cell is given by:

N = Ni + Nf/2 + Nc/8

Ni is the number of interior points
Nf is the number of points on faces
Nc is the number of points on corners

Table 3.1 Atomic Radii and Crystal Structures for 16 Metals

Metal	*Crystal Structure*[a]	*Atomic Radius*[b] *(nm)*	*Metal*	*Crystal Structure*	*Atomic Radius (nm)*
Aluminum	FCC	0.1431	Molybdenum	BCC	0.1363
Cadmium	HCP	0.1490	Nickel	FCC	0.1246
Chromium	BCC	0.1249	Platinum	FCC	0.1387
Cobalt	HCP	0.1253	Silver	FCC	0.1445
Copper	FCC	0.1278	Tantalum	BCC	0.1430
Gold	FCC	0.1442	Titanium (α)	HCP	0.1445
Iron (α)	BCC	0.1241	Tungsten	BCC	0.1371
Lead	FCC	0.1750	Zinc	HCP	0.1332

[a] FCC = face-centered cubic; HCP = hexagonal close-packed; BCC = body-centered cubic.
[b] A nanometer (nm) equals 10^{-9} m; to convert from nanometers to angstrom units (Å), multiply the nanometer value by 10.

Critical Crystal Structures:

- We have talked about point lattices and Bravais lattices -- which are topics from mathematical (geometrical) crystallography
- The Bravais lattice solutions were known well before the discovery of x-ray diffraction and any knowledge of atomic arrangement

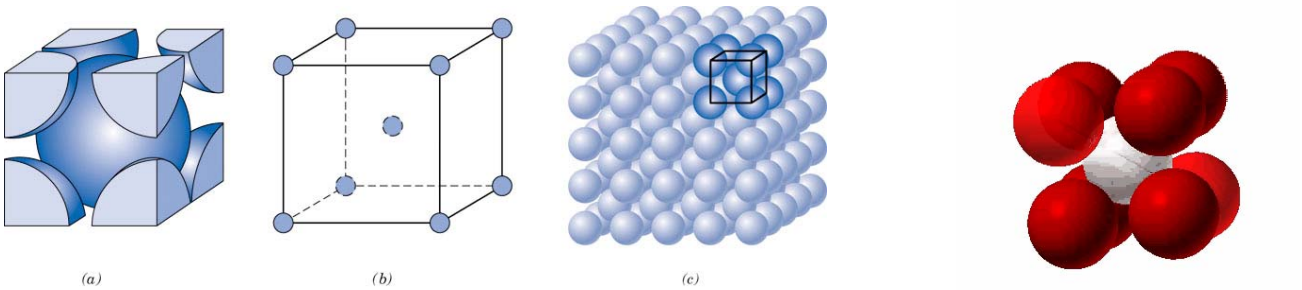
- Lets talk about some actual crystal structures of importance to material science
- Basic rule of crystal structure:
  - "*The atoms of a crystal are set in space on the points of a Bravais lattice or in some fixed relation to those points*"

- Metallic crystal structures tend to be densely packed because:
  - Typically, only one element is present, so all atomic radii are the same
  - Metallic bonding is not directional.
  - Nearest neighbor distances tend to be small in order to lower bond energy.
  - Electron cloud shields cores from each other

Body Centered Cubic -- BCC

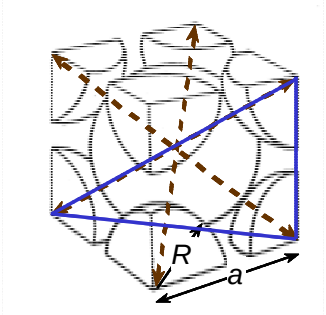
- One of the allotropic forms of iron
  - Pure Iron solidifies as δ-ferrite BCC at 1538°C
  - Transforms to γ-austenite FCC at 1394°C
  - Transforms to α-ferrite (BCC) at 912°C

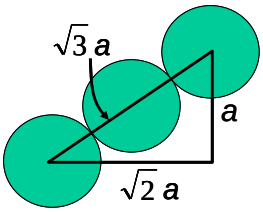
- Other Examples: Cr, W, Mo, Ta



- We have 1 atom on each of the four corners of the simple cube and 1 atom in the middle
- The atoms "touch" each other along the diagonal axes -- close packed direction
- Coordination number of the BCC cell is 8
- The number of atoms per unit cell is 2 -- use the lattice point equation
  - N = Ni + Nf/2 + Nc/8

Derivation of relationship between a -- lattice parameter and R (atomic radius)





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

- Atomic packing factor:

The sum of the spherical volumes of all atoms within the unit cell divided by the unit cell volume

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

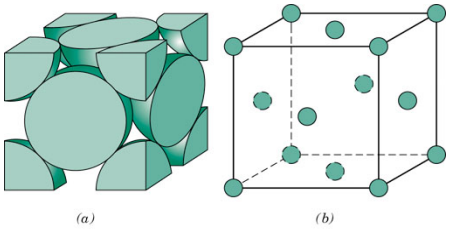
*assume hard spheres

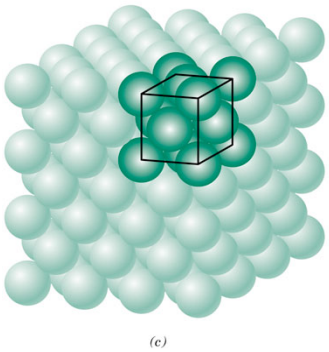
- Atomic Packing Factor for BCC is 0.68
  - Derivation on board

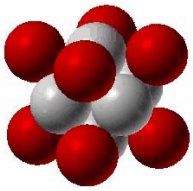
Face Centered Cubic - FCC

- Another allotropic form of iron

- Other examples include: Al, Cu, Au, Ag, Pb, Ni

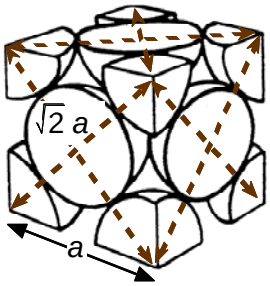






- We have 1 atom on each of the four corners of the simple cube and 1 atom in the middle of each cube face
- The atoms "touch" each other along the faces of the cube -- close packed direction
- Coordination number of the FCC cell is 12
- The number of atoms per unit cell is 4 -- use the lattice point equation
  - N = Ni + Nf/2 + Nc/8

- Derivation of relationship between a and R:

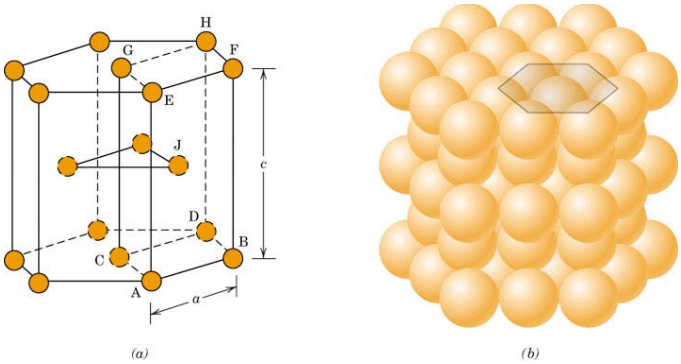


Close-packed directions:
length = $4R = \sqrt{2}\,a$

- Atomic packing factor for FCC is 0.74

Hexagonal Close Pack -- HCP

- Examples include: Ti, Zn, Cd, Co



- Not cubic -- but hexagonal symmetry
- Top and bottom faces of unit cell consist of 6 atoms that form regular hexagons and surround 1 atom in center
- Mid-plane provides additional 3 atoms to unit cell is between top and bottom
- The number of atoms per unit cell is 6
  - 1/6 of each of the 12 top and bottom atoms
  - 1/2 of each of the center atoms from top and bottom planes
  - 3 center atoms
- Coordination number is 12 (same as FCC)
- Atomic Packing factor is 0.74 (same as FCC)