

MEAM/MSE 507

Fundamentals of Materials

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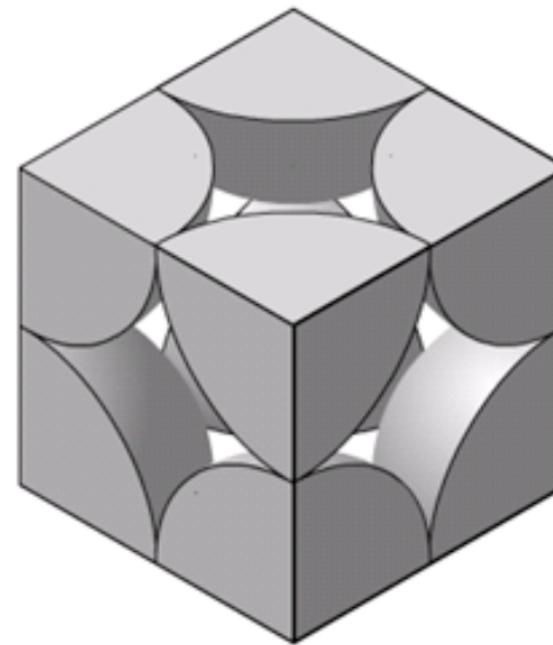
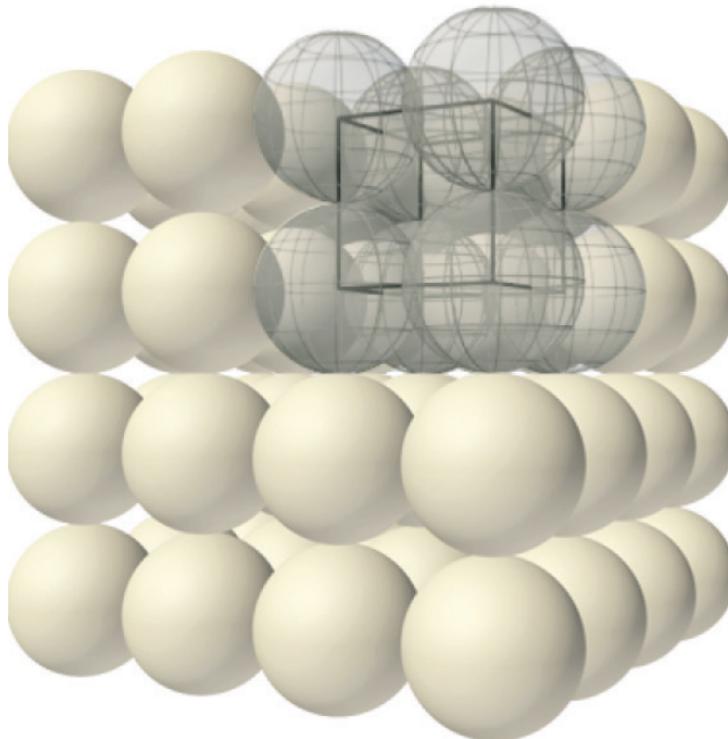
Week 5, Lecture 1: Physical crystals (part 1)
Asynchronous

Metallic crystal structures

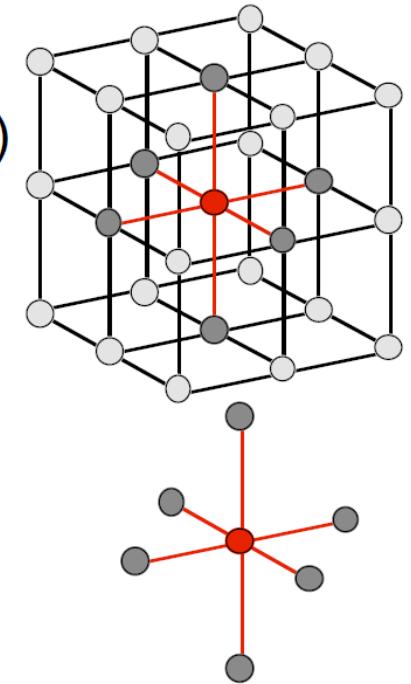
- Tend to be densely packed
- Reasons for dense packing:
 - Typically, only one element is present or atoms are of similar size
 - Metallic bonding is non-directional (predominantly)
 - Nearest neighbor distances tend to be small in order to lower bond energy
 - Electron cloud shields cores from each other
- Metals have the simplest crystal structures

Simple cubic structure (SC)

- Rare due to low packing density (only Po has this structure)
- Close-packed directions are cube edges.



- Coordination # = 6
(# nearest neighbors)



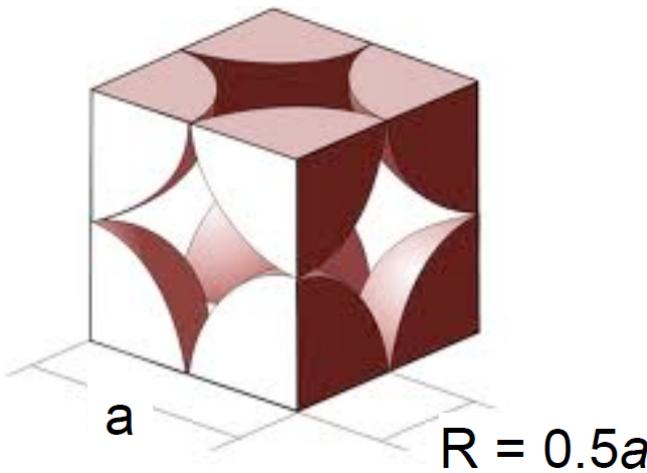
Octahedral symmetry

Atomic packing factor (APF)

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

*assume hard spheres

- APF for a simple cubic structure = 0.52



$$APF = \frac{\frac{\text{atoms}}{\text{unit cell}} \times \frac{\text{volume}}{\text{atom}}}{\frac{\text{volume}}{\text{unit cell}}}$$

$$= \frac{1 \times \frac{4}{3} \pi (0.5a)^3}{a^3}$$

Cube edges are the close-packed directions

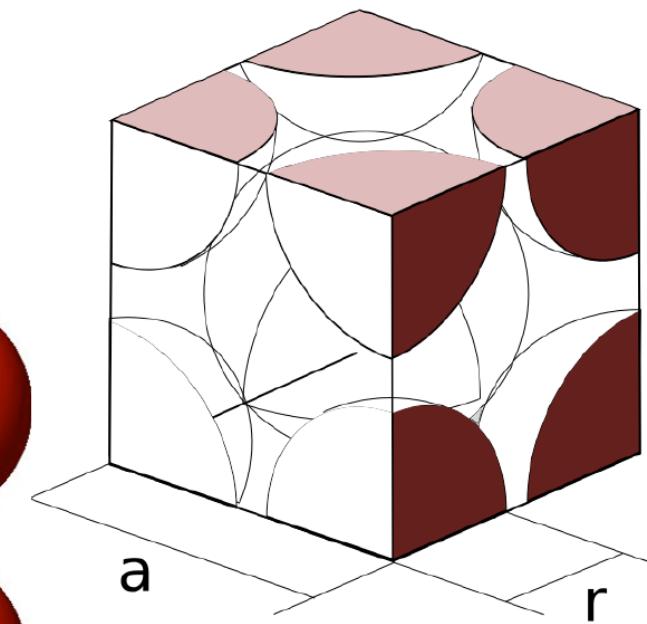
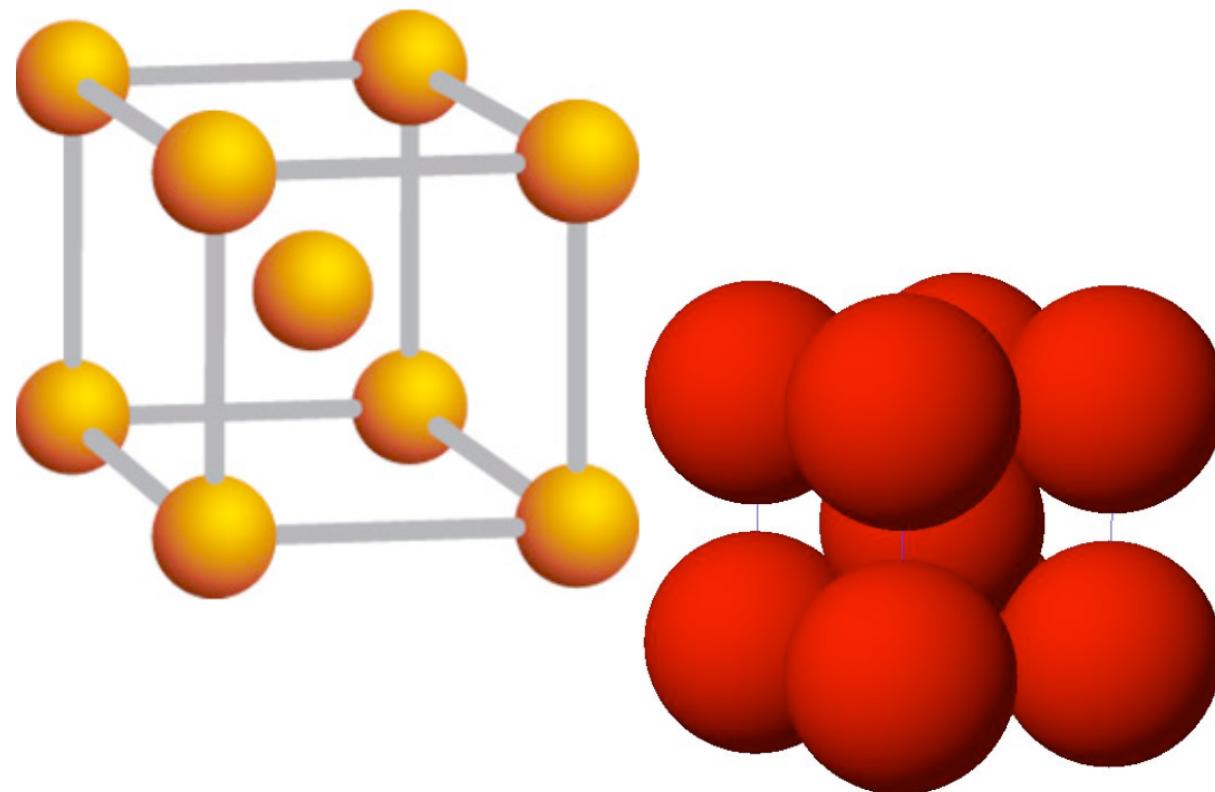
contains $8 \times 1/8 =$

1 atom/unit cell

- APF for a simple cubic structure = 0.52

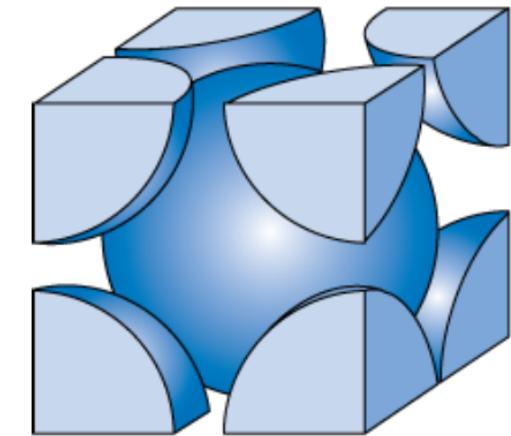
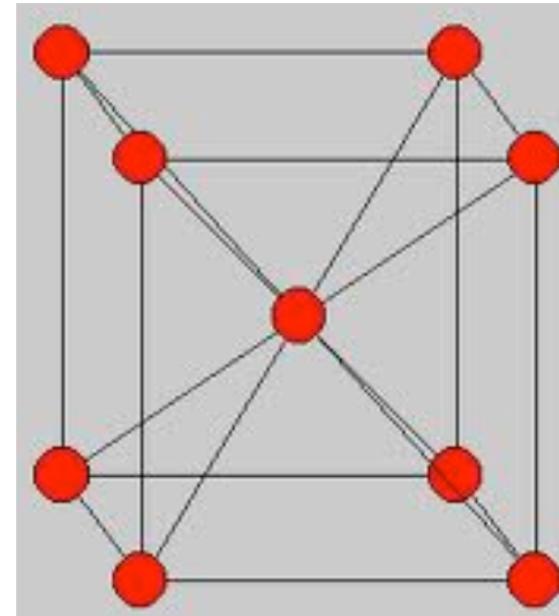
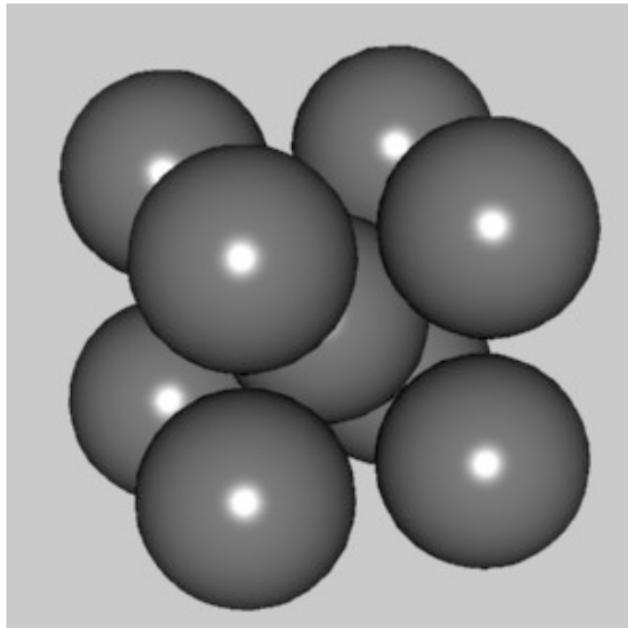
Body centered cubic (BCC)

- Simple Cubic with an extra atom in the center of the (body) unit cell



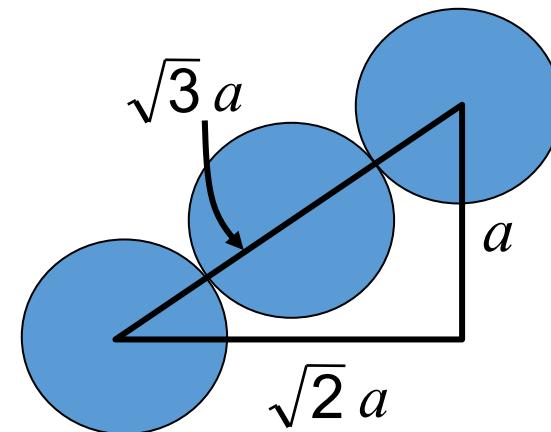
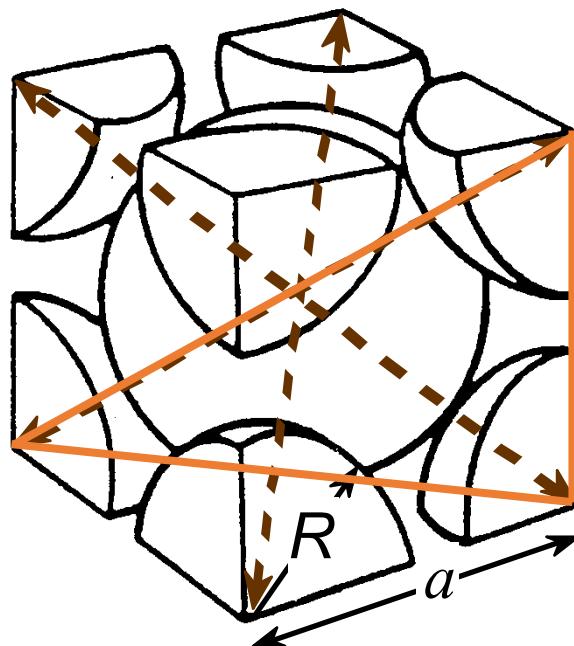
Body centered cubic (BCC)

examples: Cr, W, Fe (α), Tantalum, Molybdenum



2 atoms/cubic unit cell: 1 center + 8 corners $\times \frac{1}{8}$

Atomic packing factor: BCC



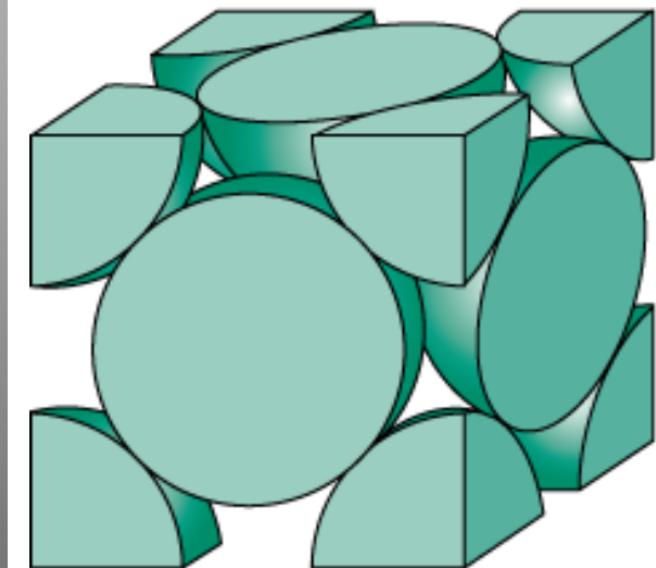
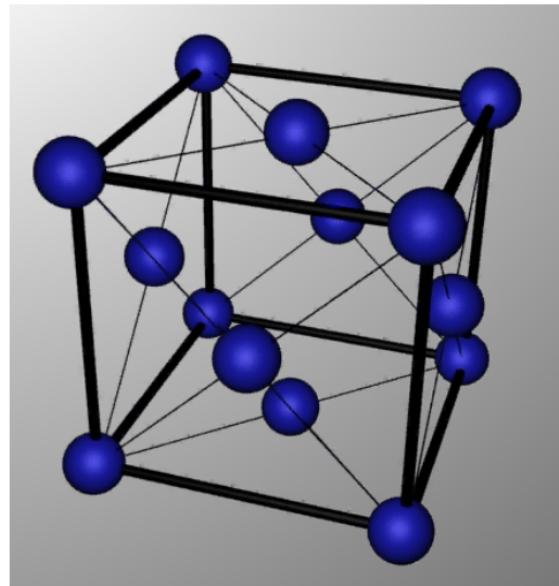
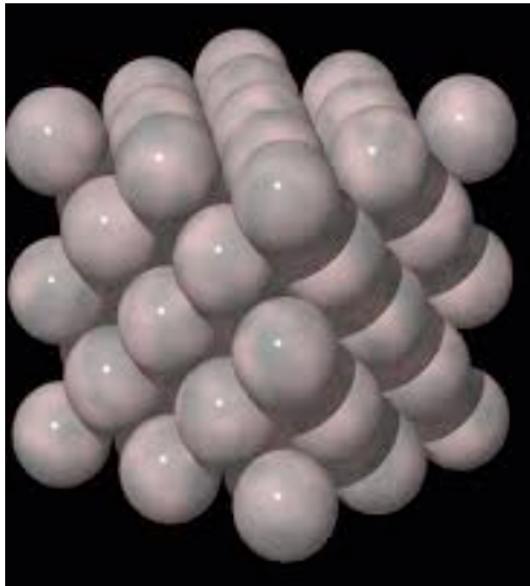
Close-packed directions:
length = $4R = \sqrt{3} a$

$$APF = \frac{\frac{atoms}{unit\ cell} \cdot \frac{4}{3} \pi (\sqrt{3}a/4)^3}{\frac{volume}{unit\ cell} \cdot a^3}$$

- APF for a body-centered cubic structure = 0.68

Face centered cubic (FCC)

examples: Al, Cu, Au, Pb, Ni, Pt, Ag



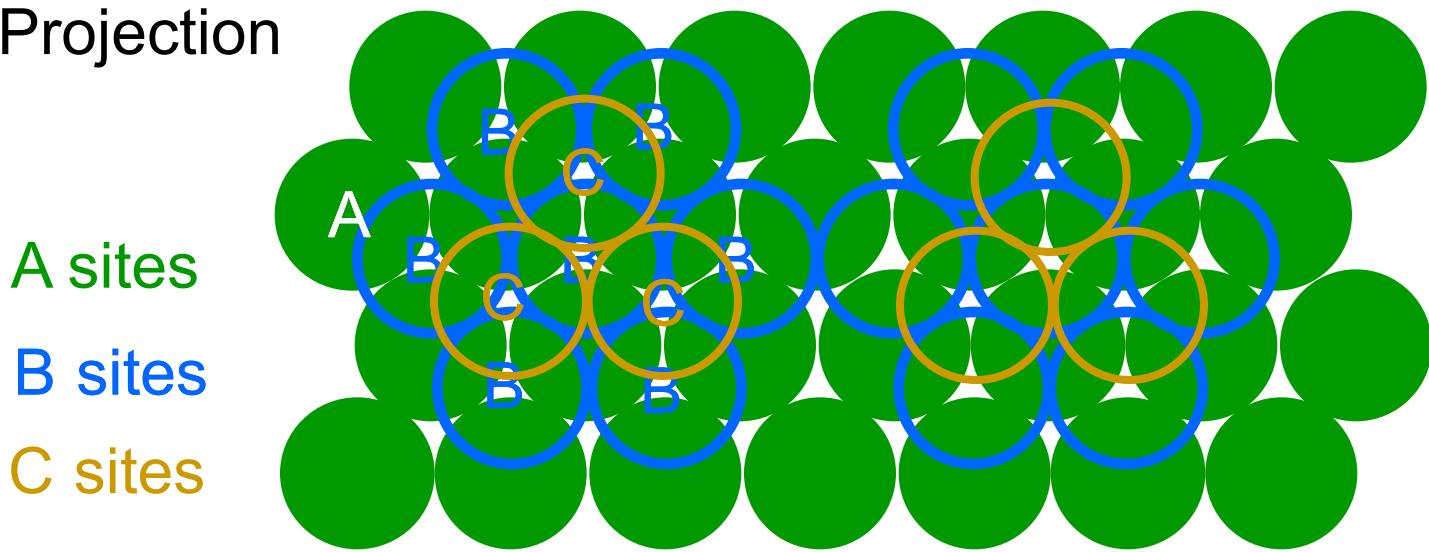
Coordination # = 12

Atoms touch along
face diagonals

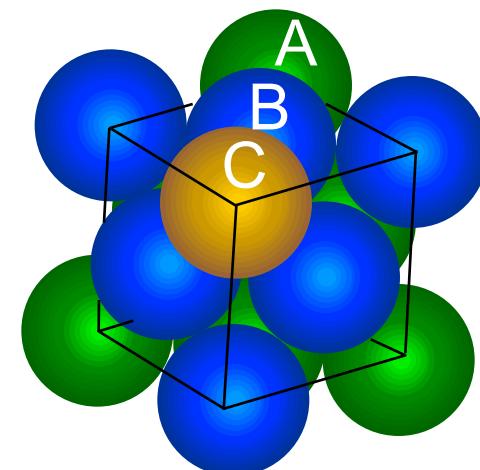
4 atoms/unit cell: $6 \text{ face} \times 1/2 + 8 \text{ corners} \times 1/8$

FCC stacking sequence

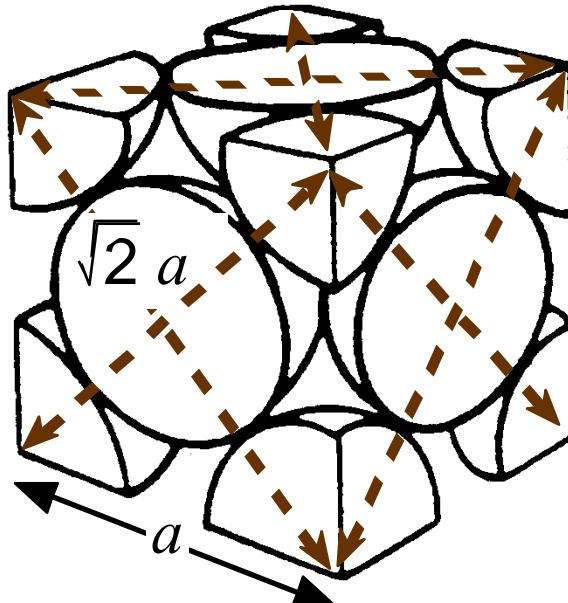
- ABCABC... Stacking Sequence
- 2D Projection



- FCC Unit Cell



Atomic packing factor: FCC



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

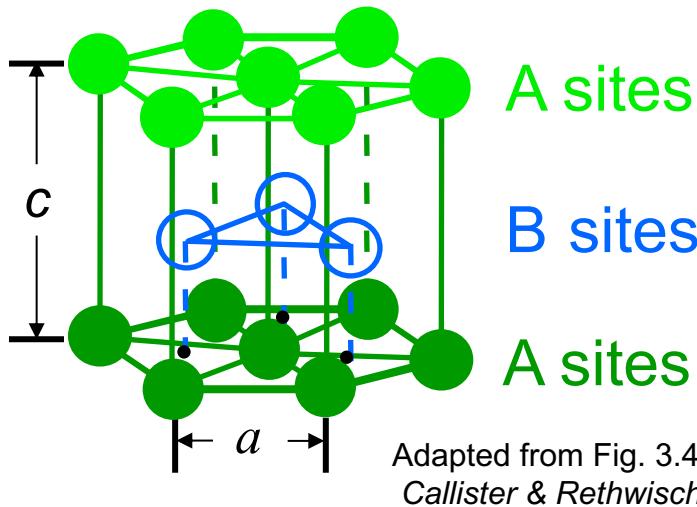
Unit cell contains:
 $6 \times 1/2 + 8 \times 1/8$
= **4 atoms/unit cell**

$$\text{APF} = \frac{\frac{\text{atoms}}{\text{unit cell}}}{\frac{\text{volume}}{\text{unit cell}}} = \frac{4}{\frac{4}{3} \pi (\sqrt{2}a/4)^3}{\frac{\text{volume}}{\text{atom}}}$$

- APF for a face-centered cubic structure = 0.74
- Highest possible APF

Hexagonal close-packed (HCP)

- ABAB... Stacking Sequence
- 3D Projection



- 2D Projection

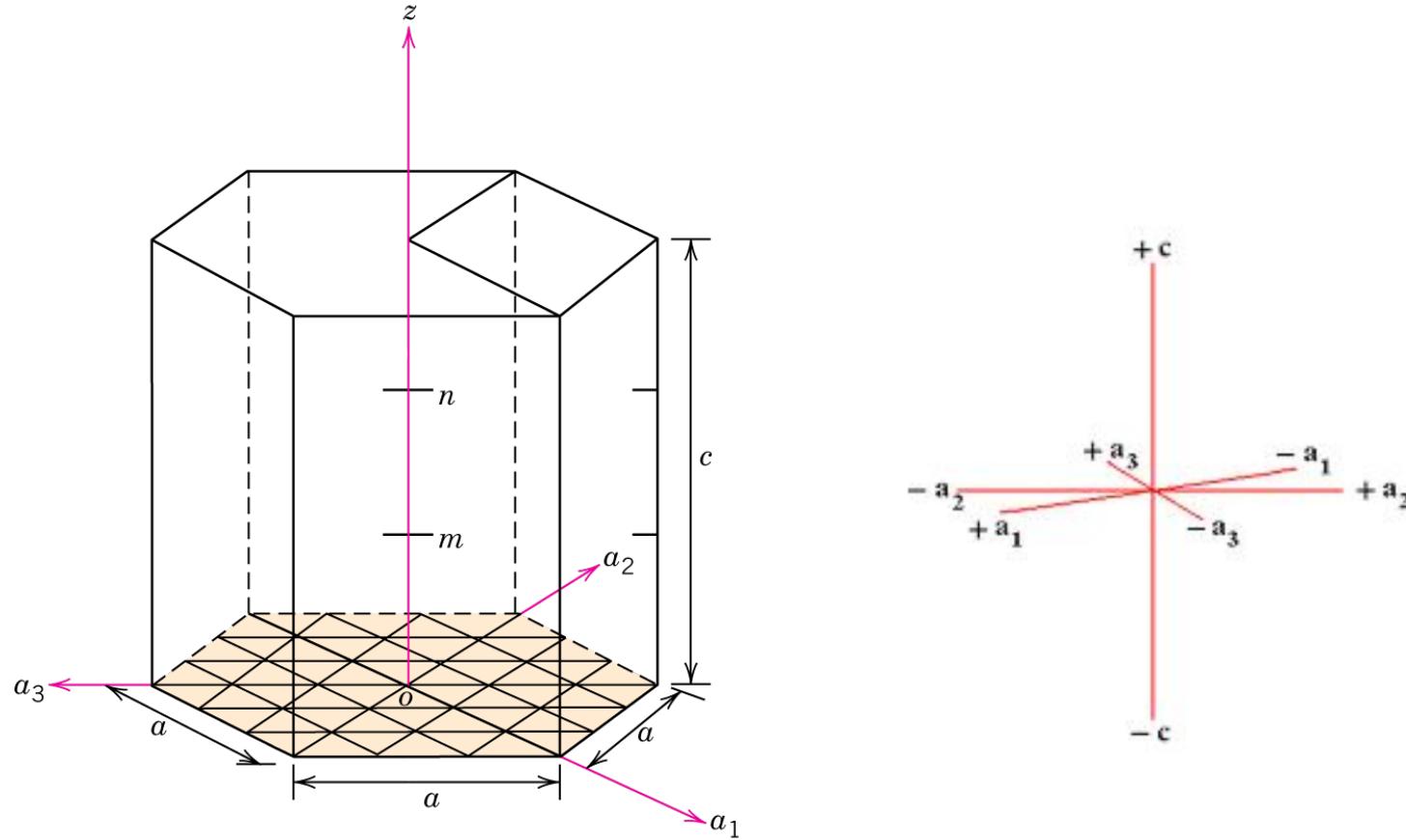


- Coordination # = 12
- APF = 0.74
- $c/a = 1.633$

6 atoms/unit cell

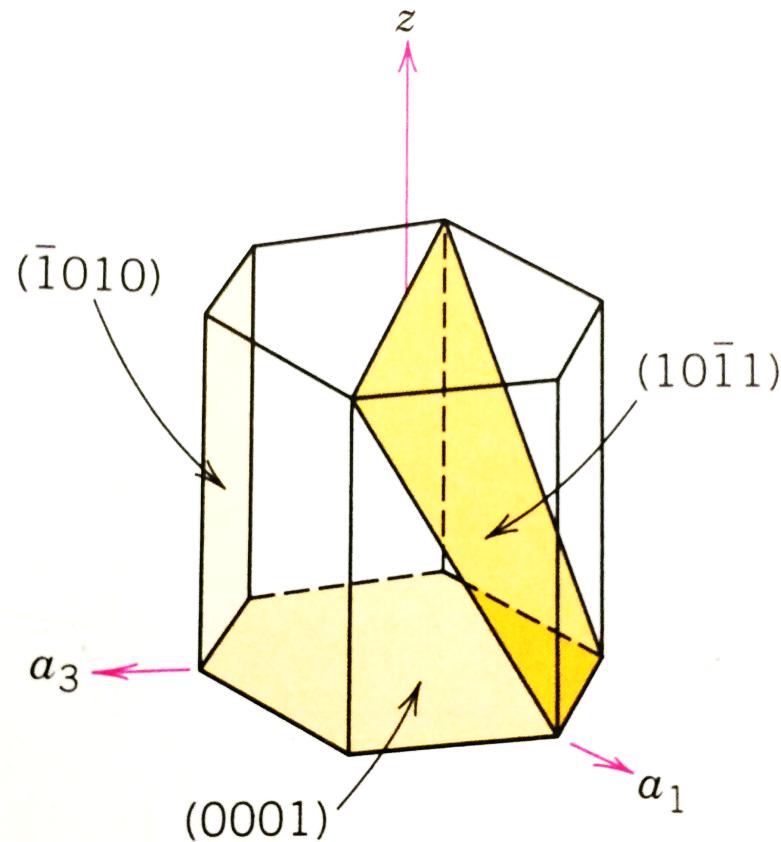
ex: Cd, Mg, Ti, Zn

HCP crystallography



- Though only 3 coordinates would still be required for HCP, the symmetry of the system makes it more convenient to use 4.
- The 4 indices ($uvtw$) lie parallel with a_1 , a_2 , a_3 , and c directions, respectively
- t is redundant: $t=-(u+v)$

Miller indices in hexagonal lattices



Miller indices in hexagonal lattices

EXAMPLE PROBLEM 3.13

Determination of the Miller–Bravais Indices for a Plane within a Hexagonal Unit Cell

Determine the Miller–Bravais indices for the plane shown in the hexagonal unit cell.

Solution

These indices may be determined in the same manner that was used for the x - y - z coordinate situation and described in Example Problem 3.11. However, in this case the a_1 , a_2 , and z axes are used and correlate, respectively, with the x , y , and z axes of the previous discussion. If we again take A , B , and C to represent intercepts on the respective a_1 , a_2 , and z axes, normalized intercept reciprocals may be written as

$$\frac{a}{A} \quad \frac{a}{B} \quad \frac{c}{C}$$

Now, because the three intercepts noted on the above unit cell are

$$A = a \quad B = -a \quad C = c$$

values of h , k , and l , may be determined using Equations 3.14a–3.14c, as follows (assuming $n = 1$):

$$h = \frac{na}{A} = \frac{(1)(a)}{a} = 1$$

$$k = \frac{na}{B} = \frac{(1)(a)}{-a} = -1$$

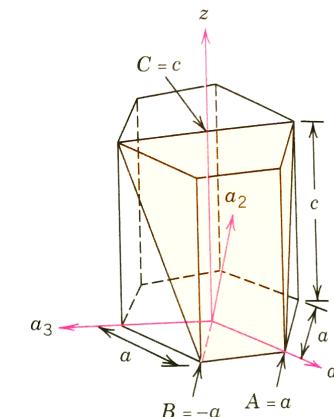
$$l = \frac{nc}{C} = \frac{(1)(c)}{c} = 1$$

And, finally, the value of i is found using Equation 3.15, as follows:

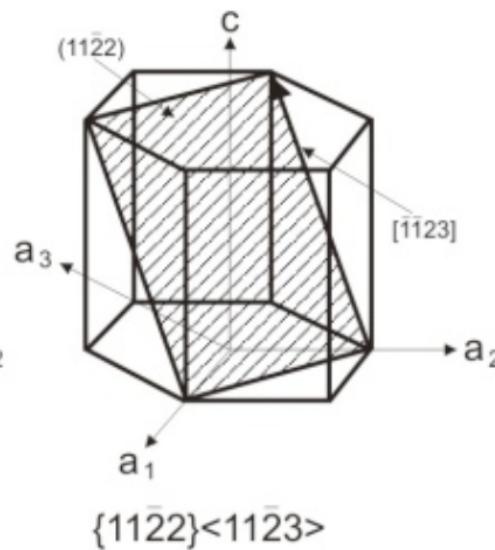
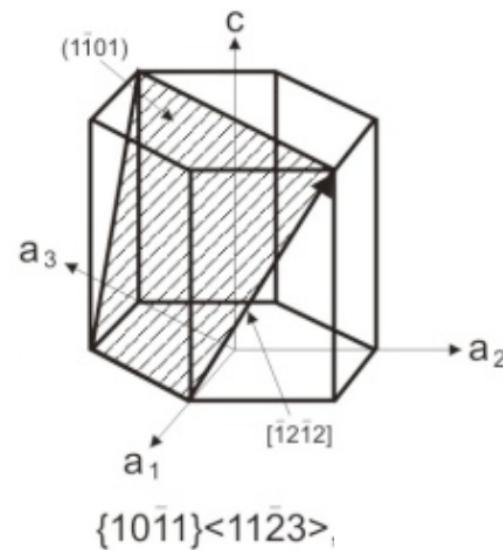
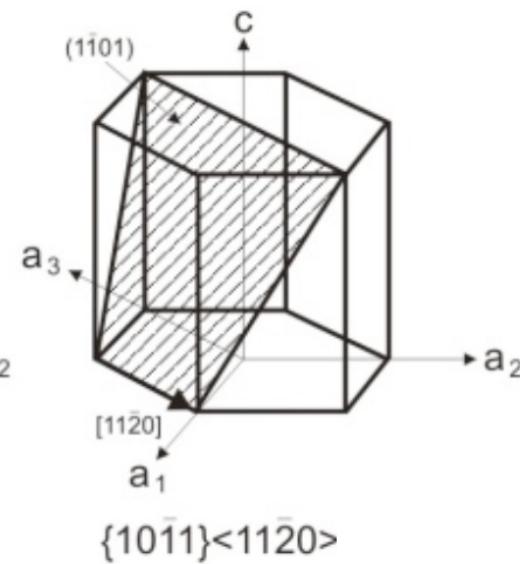
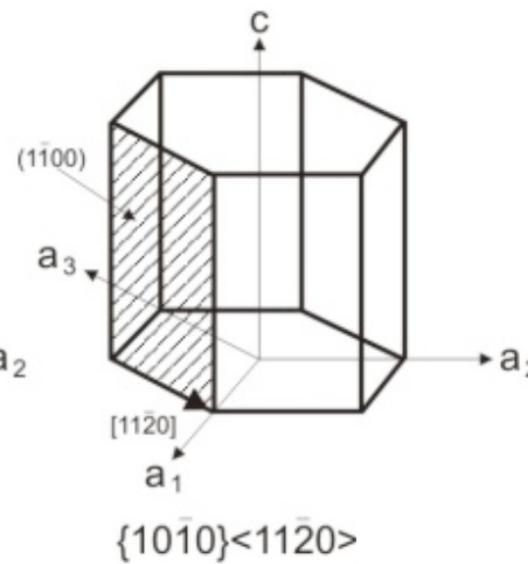
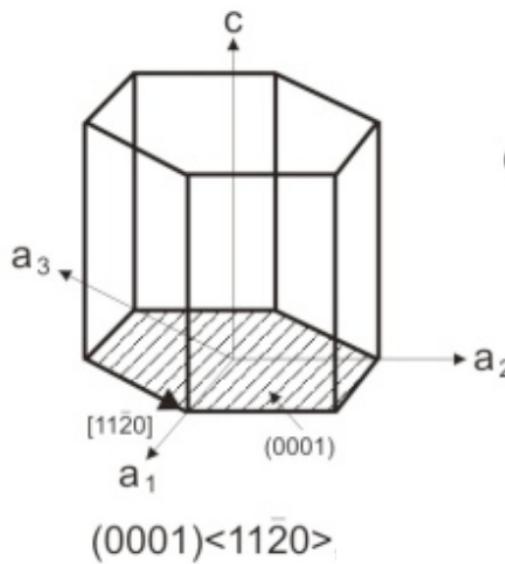
$$i = -(h + k) = -[1 + (-1)] = 0$$

Therefore, the $(hkil)$ indices are $(1\bar{1}01)$.

Notice that the third index is zero (i.e., its reciprocal $= \infty$), which means this plane parallels the a_3 axis. Inspection of the preceding figure shows that this is indeed the case.



HCP crystallography



{ } – Family of planes
 <> - Family of directions