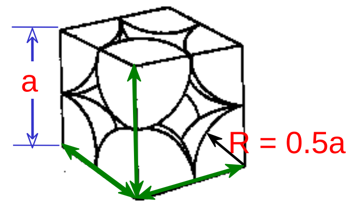
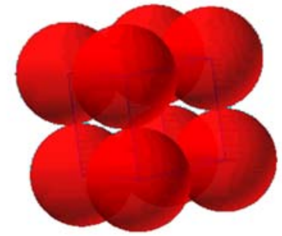
Outline:

- Review of Crystal structure
- Stacking Sequence
- Theoretical Density
- Crystallographic Directions and Planes
  - *examples*

Review: *Crystal Structure*

- Close-packed directions are ……………

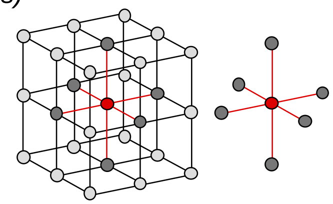




This is a …. unit cell

- Contains = …………………
- Coordination # = …. *(# nearest neighbors)*

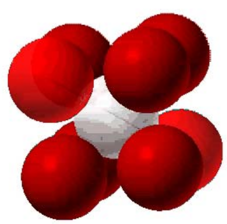
$$\text{APF} = \frac{1 \; \frac{4}{3}\pi (0.5a)^3}{a^3}$$



- APF for a simple cubic structure = ………

Review: *Crystal Structure*

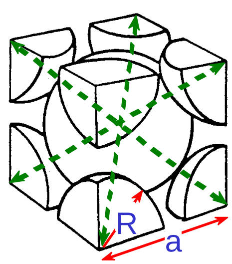
- Close packed directions are ……………………
- Coordination # = ……



Note: *All atoms are identical; the center atom is shaded differently only for ease of viewing.*

This is a …... unit cell

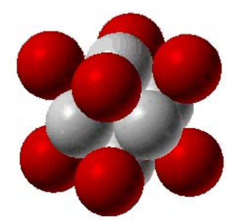
$$\text{APF} = \frac{2 \; \frac{4}{3}\pi (\sqrt{3}a/4)^3}{a^3}$$



- APF for a BCC structure = …….

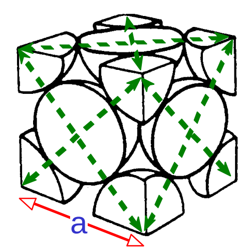
Review: *Crystal Structure*

- Close packed directions are ………………..
- Coordination # = ……..



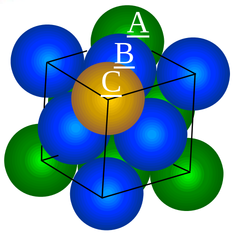
This is a ….... unit cell

$$\text{APF} = \frac{4 \; \frac{4}{3}\pi (\sqrt{2}a/4)^3}{a^3}$$

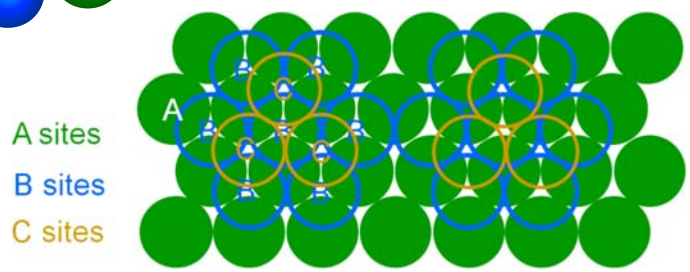


- APF for a FCC structure = ……

FCC Stacking Sequence



• FCC Unit Cell



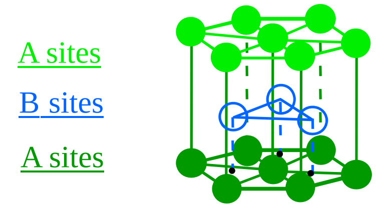
2D Projection

• ABCABC... Stacking Sequence

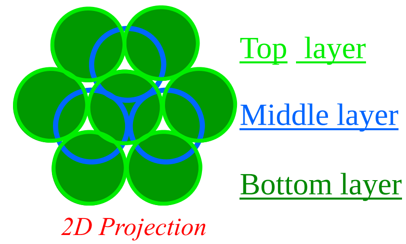
Review: *Crystal Structure*

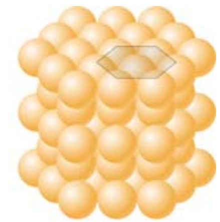
• Coordination # = ……

• APF = ………



This is a …... unit cell





• Stacking Sequence: …………

Example Problem

- If you know
  - the crystal structure,
  - the atomic radius
  - the atomic weight,

you can calculate the density of a particular material

Example:

Copper has an atomic radius 0.128 nm an FCC crystal structure and an atomic weight of 63.5 g/mol. Calculate its density.

Crystallographic Directions, and Planes

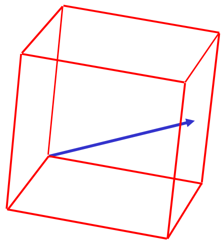
Now that we know how atoms arrange themselves to form crystals, *we need a way to identify directions and planes of atoms.*

•Why?

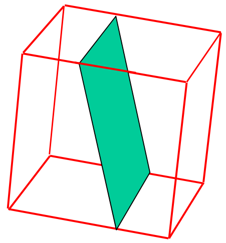
✓ Deformation under loading (*slip*) occurs on certain crystalline planes and in certain crystallographic directions. Before we can predict how materials fail, we need to know what modes of failure are more likely to occur.

✓ Other properties of materials (*electrical conductivity, thermal conductivity, elastic modulus*) can vary in a crystal with orientation.

Crystallographic Planes & Directions



direction



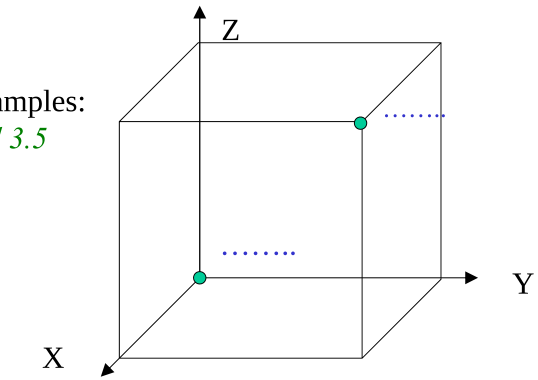
plane

- It is often necessary to be able to specify certain directions and planes in crystals.
- Many material properties and processes vary with direction in the crystal.
- Directions and planes are described using three integers - ………. Indices

Point coordinates

- Point position specified in terms of its coordinates as fractional multiples of the unit cell edge lengths

See examples:
3.4 and 3.5



General Rules for Lattice Directions, Planes & Miller Indices

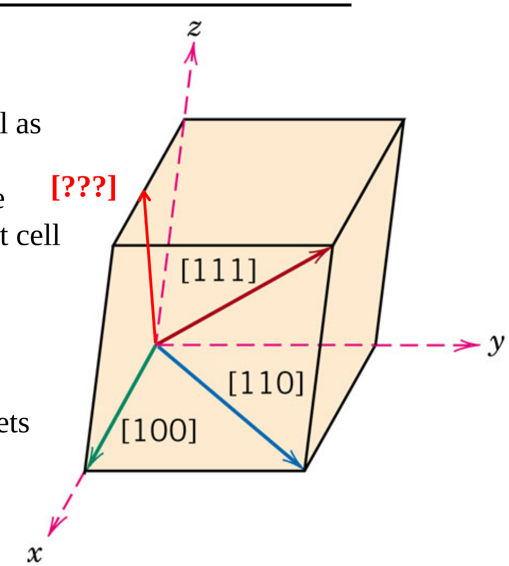
- Miller indices used to express lattice *planes* and *directions*
- x, y, z are the axes (on arbitrarily positioned origin)
  - *in some crystal systems these are not mutually ⊥*
- a, b, c are lattice parameters (*length of unit cell along a side*)
- h, k, l are the Miller indices for planes and directions - expressed as planes: (hkl) and directions: [hkl]
- Conventions for naming
  - There are NO COMMAS between numbers
  - Negative values are expressed with a bar over the number
    - *Example:* *-2 is expressed* $\bar{2}$

- Crystallographic direction:
  - [123]
  - [100]
  - … etc.

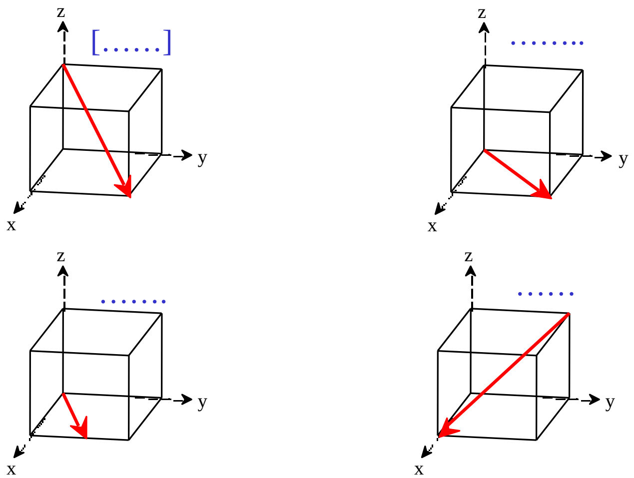
Miller Indices for Directions

Method

- Draw vector, define tail as origin.
- Determine length of the vector projection in unit cell dimensions, a, b, and c
- Remove fractions by multiplying by smallest possible factor
- Enclose in square brackets
- What is ???

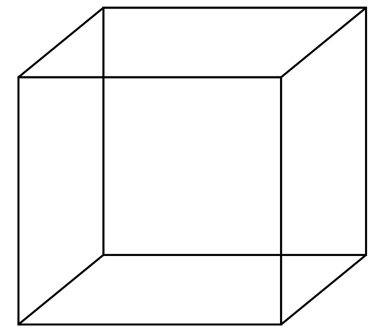


Example - Naming Directions



Example - Drawing Directions

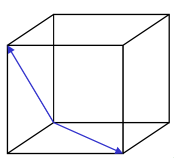
- Draw [1 1 $\bar{2}$] and [$\bar{1}\,\bar{1}\,\bar{1}$]



The HW problems will give you more practice with directions

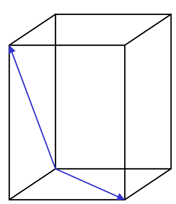
Families of Directions

- Equivalence of directions



[101] = [110]

cubic



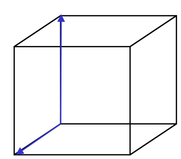
[101] ≠ [110]

tetragonal

- <123> Family of directions
  - [123], [213], [312], [132], [231], [321]
    - *– only in a cubic crystal*

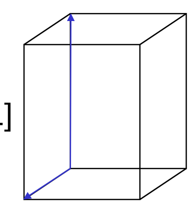
*In the cubic system directions having the same indices regardless of **order** or **sign** are equivalent.*

Isotropy vs. Anisotropy in Single Crystals



[100] = [001]

cubic



[100] ≠ [001]

tetragonal

....

- Properties are independent of direction → isotropic material
- Directionality of properties → anisotropic material

Miller Indices for Planes

- (hkl) Crystallographic plane
- {hkl} Family of crystallographic planes
  - e.g. (hkl), (lhk), (hlk) … etc.

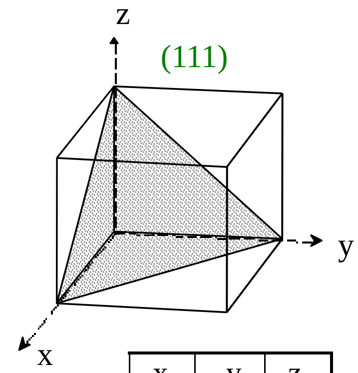
*In the cubic system planes having the same indices regardless of **order** or **sign** are equivalent*

- Hexagonal crystals can be expressed in a four index system (u v t w)
  - *Can be converted to a three index system using formulas*

Miller Indices for ***PLANES***

Method

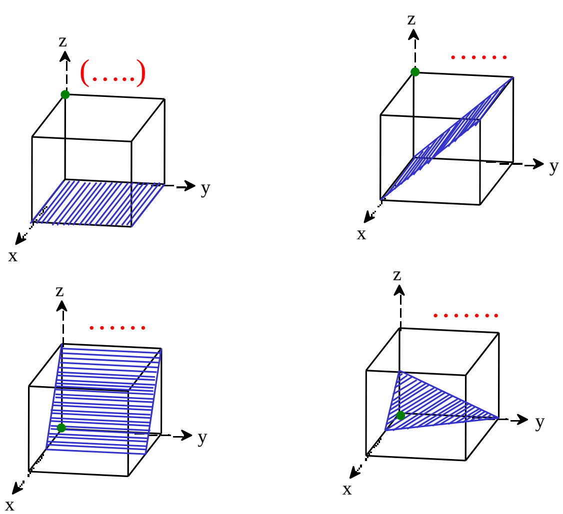
- If the plane passes through the origin, select an equivalent plane or move the origin
- Determine the intersection of the plane with the axes in terms of a, b, and c
- Take the reciprocal *(1/∞ = 0)*
- Convert to smallest integers *(optional)*
- Enclose by parentheses



	x	y	z
Intercepts			
Reciprocals			

see example 3.8

Crystallographic Planes



Next time:

Linear and Planner Densities