ENGG 201 - Chapter 3 – Bravais Lattices + Solid Density

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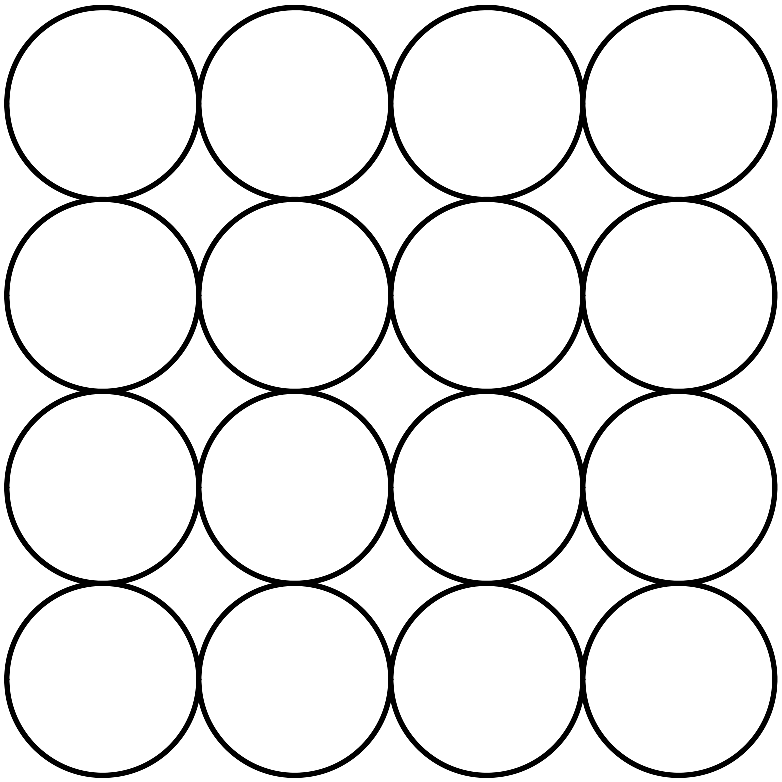
Solids

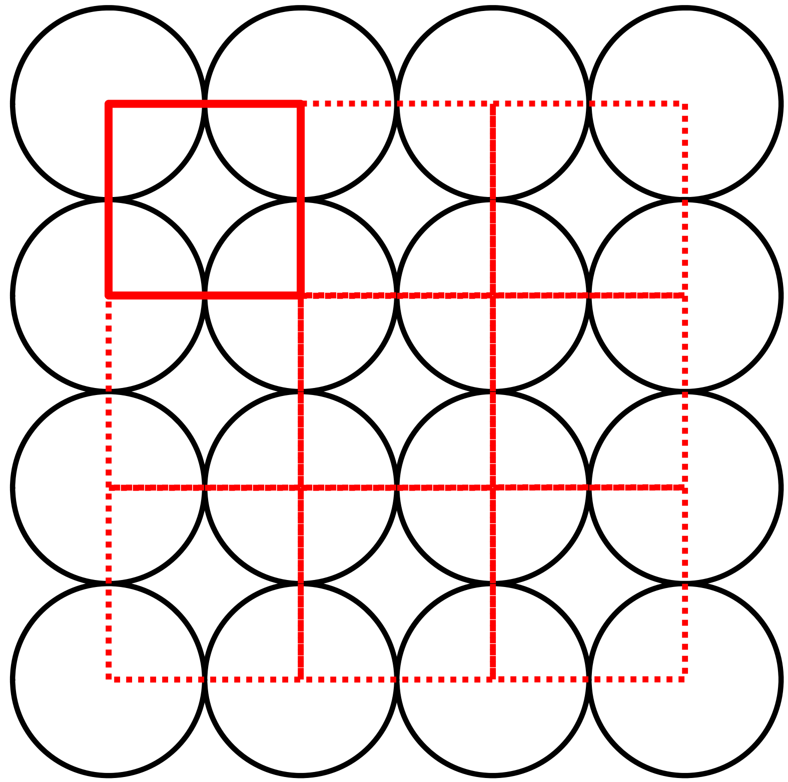
- Crystalline solids have a high degree of organization in the arrangement of their atoms/molecules
- Same arrangement repeats in all 3 directions
- Smallest repeating unit that can be used to make this arrangement is called the "unit cell"
- Unit cell = box

Unit Cell (2D Example)

Simple pattern of packed molecules:



Unit Cell (dark square):



Bravais Lattice Basics (1)

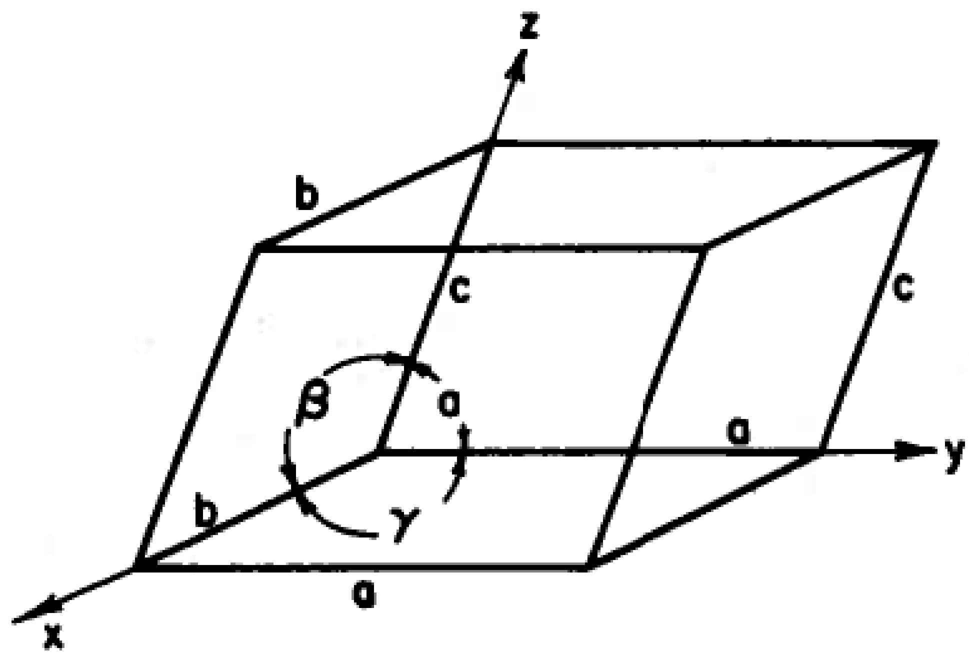


Figure 3-9 Axes in Crystals

- Different angles
- Different side lengths

Bravais Lattice Basics (2)

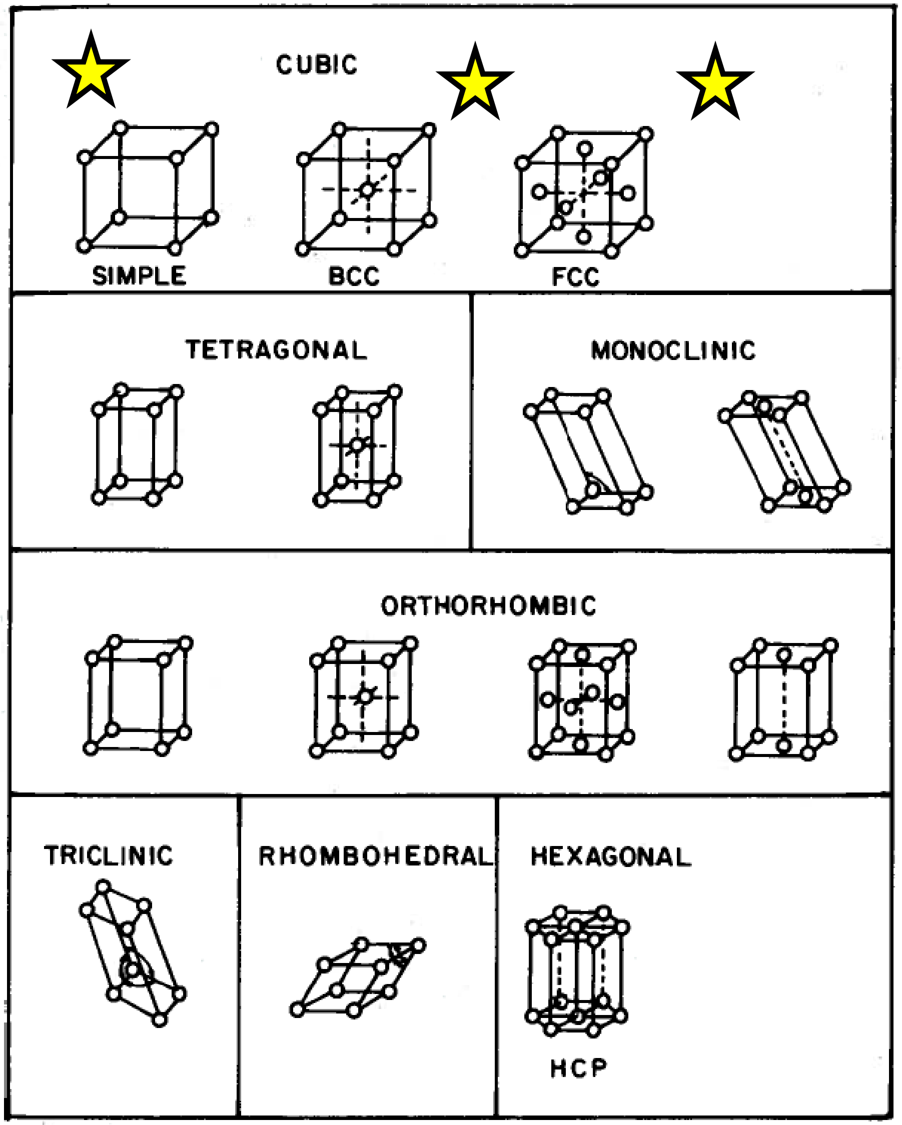
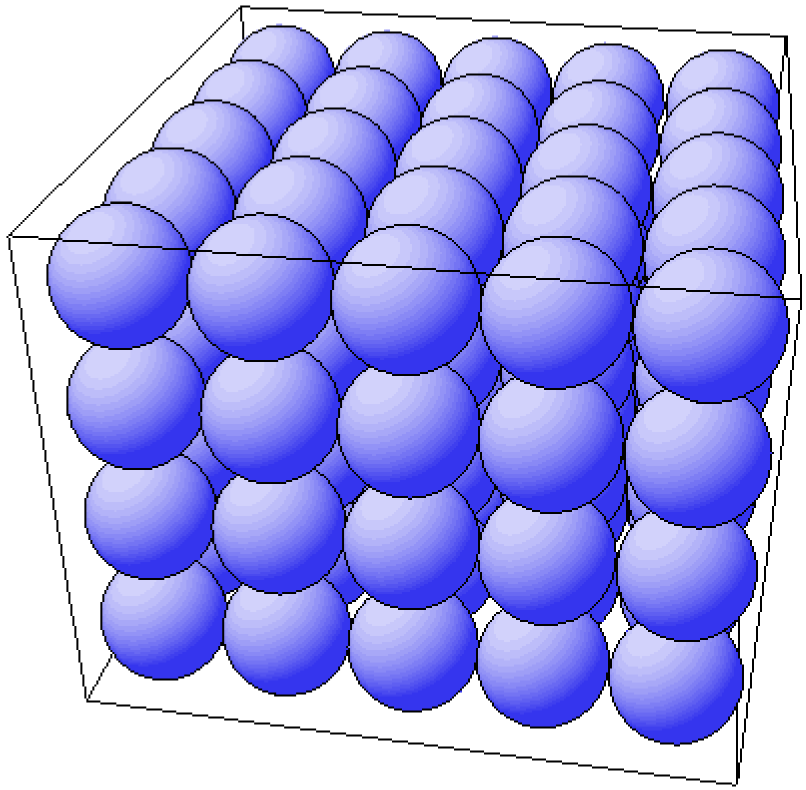


Figure 3-10 The Fourteen Bravais Lattices

Table 3-7 The Fourteen Bravais Lattices

System	Lengths of Sides	Angles Between Surfaces
Cubic		
Simple Face-Centered Body-Centered	$a = b = c$	$\alpha = \beta = \gamma = 90°$
Rhombohedral	$a = b = c$	$\alpha = \beta = \gamma \neq 90°$
Triclinic	$a \neq b \neq c$	$\alpha \neq \beta \neq \gamma$
Monoclinic		
Simple Base-Centered	$a \neq b \neq c$	$\alpha = \gamma = 90° \neq \beta$
Orthorhombic		
Simple Base-Centered Body-Centered Face-Centered	$a \neq b \neq c$	$\alpha = \beta = \gamma = 90°$
Tetragonal		
Simple Body-Centered	$a = b \neq c$	$\alpha = \beta = \gamma = 90°$
Hexagonal	$a \neq c$	$\alpha = \beta = 90°, \gamma = 120°$

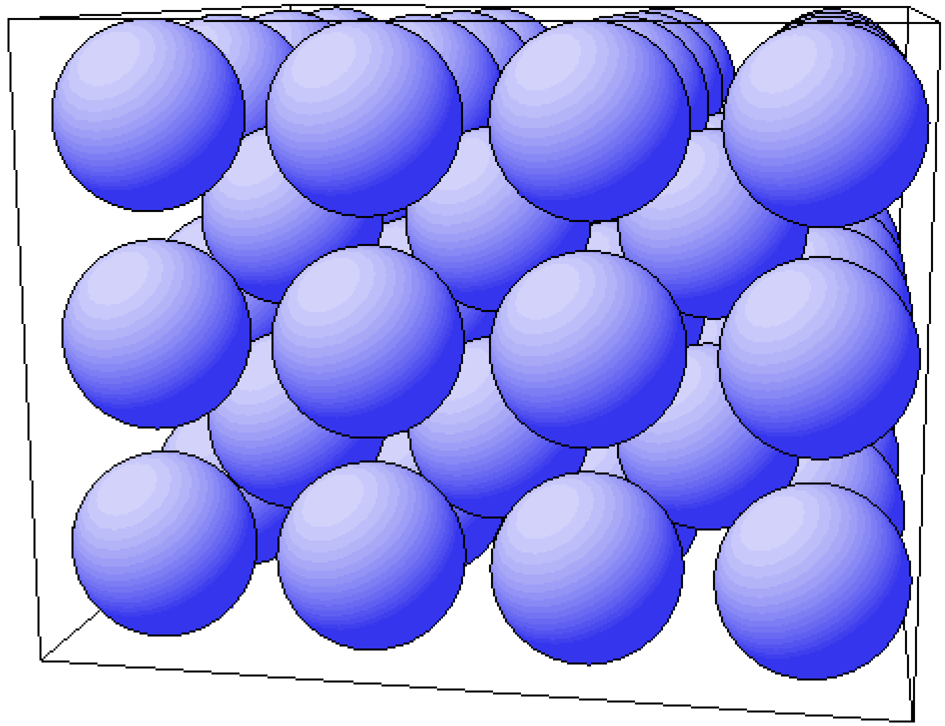
Simple Cubic



(0 0 1) Simple cubic (sc)

http://www.cmmp.ucl.ac.uk/~ijf/3c25/fcc101.gif

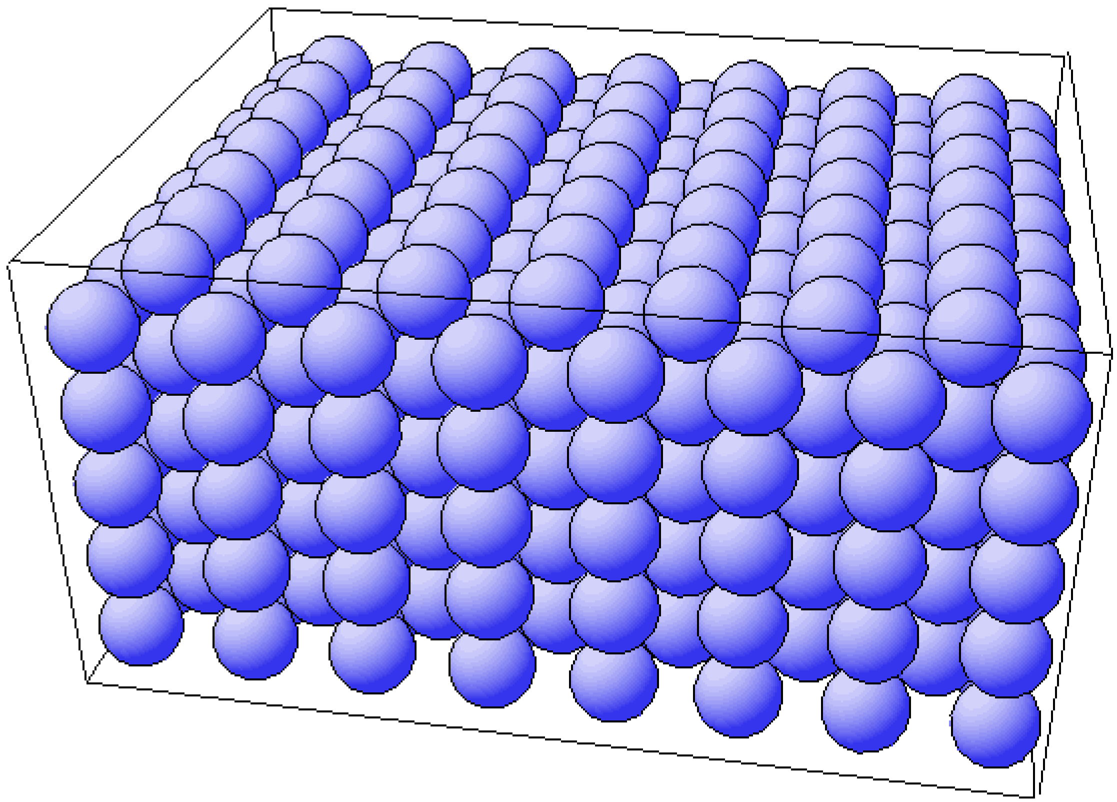
Body Centered Cubic (BCC)



(0 0 1)c Body centered cubic (bcc)

http://www.cmmp.ucl.ac.uk/~ijf/3c25/fcc101.gif

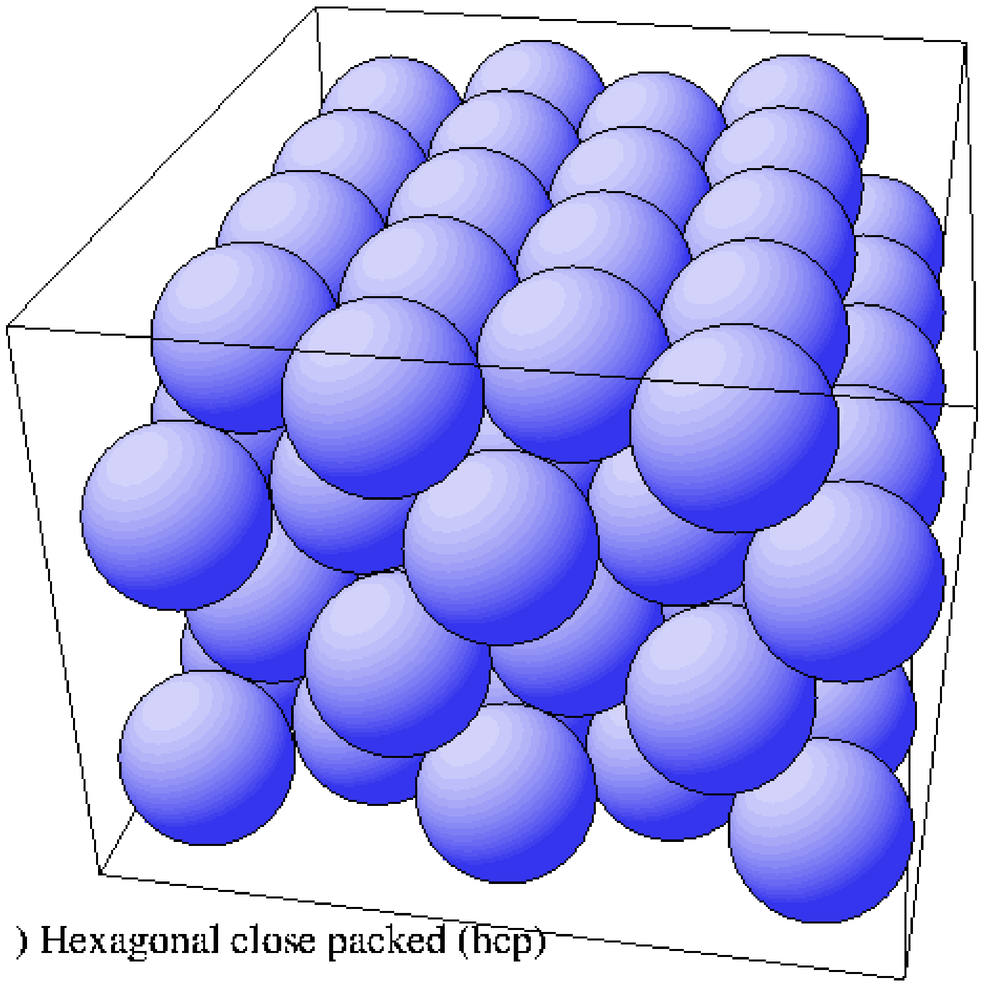
Face Centered Cubic (FCC)



(1 0 1)c Face centered cubic (fcc)

http://www.cmmp.ucl.ac.uk/~ijf/3c25/fcc101.gif

Hexagonal Close Packing (HCP)



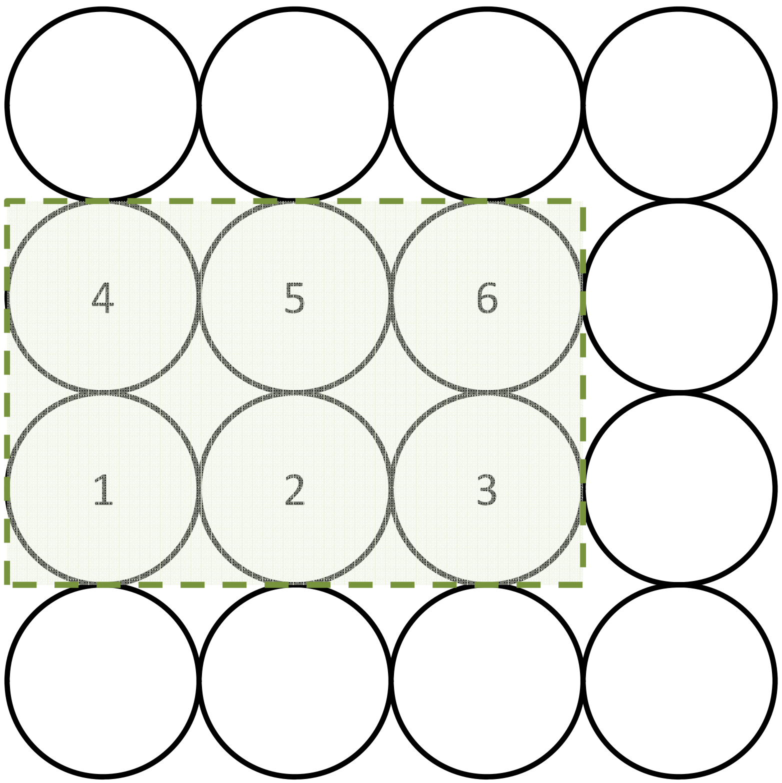
(0 0 1) Hexagonal close packed (hcp)

HCP Density the same as FCC

http://www.cmmp.ucl.ac.uk/~ijf/3c25/fcc101.gif

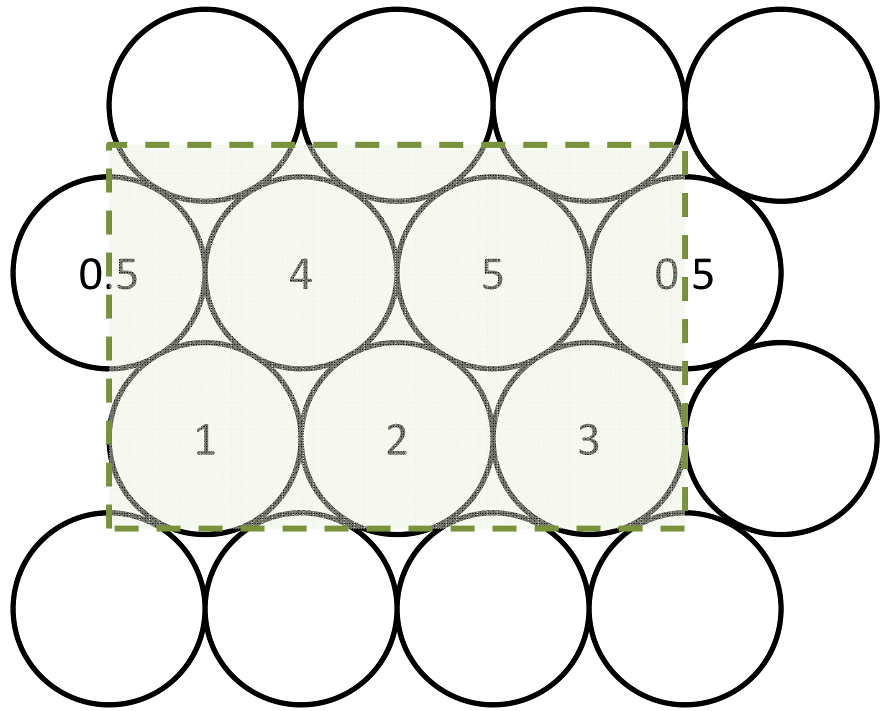
Atomic Dimensions and Density

- Packing of Molecules Influences Density (number of molecules in a given volume)



6 molecules

vs.

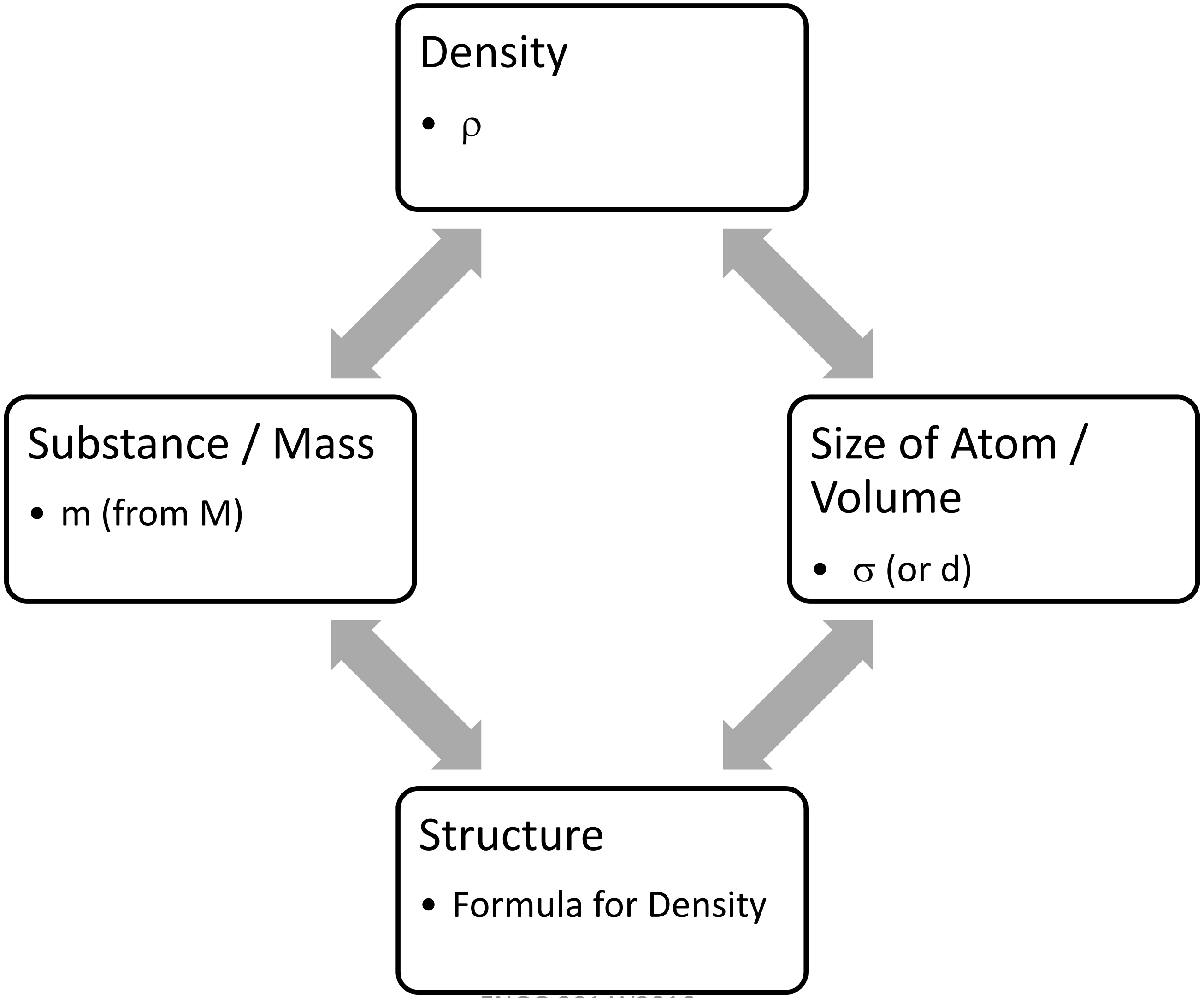


> 6 molecules

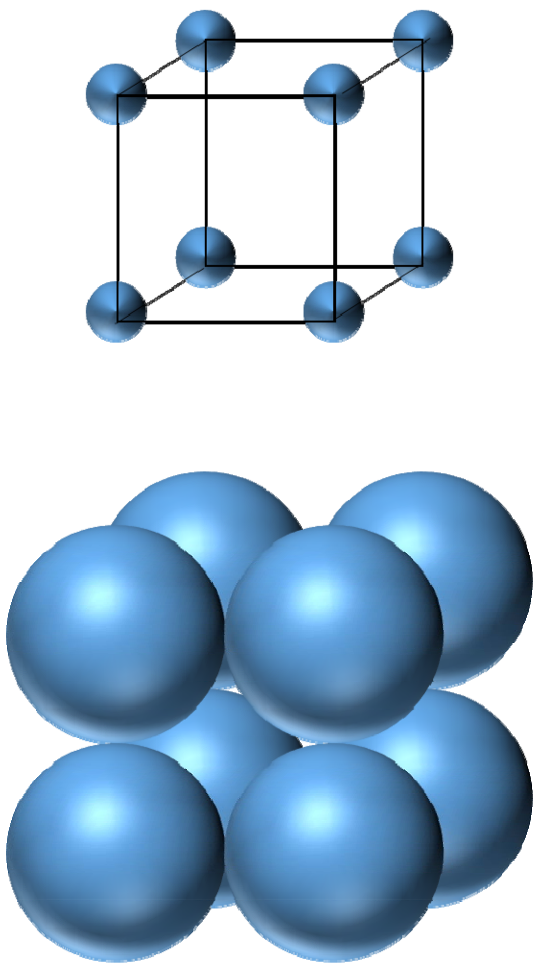
Atomic Dimensions and Density

- Use the Unit Cell as a basis
  - Mass
    - Know the mass of each atom
    - Know the number of atoms in a unit cell
  - Volume
    - Know size of the molecules
    - Know the size of the unit cell (based on packing arrangement)
- We can calculate the density of the solid
  - Density of unit cell = Density of bulk solid
  - Density = mass/volume

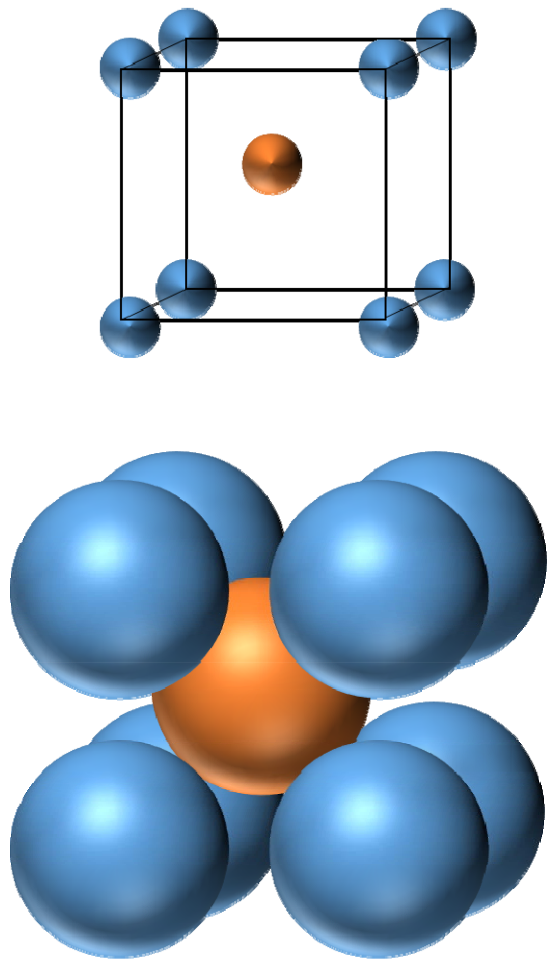
Relationship Between Variables



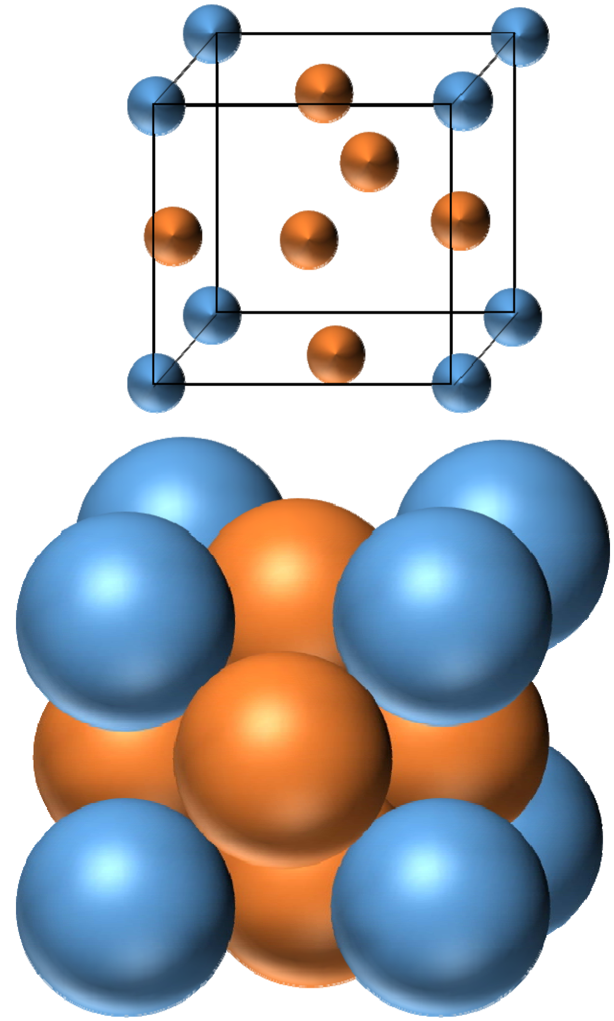
Three Cubic Arrangements



Simple Cubic

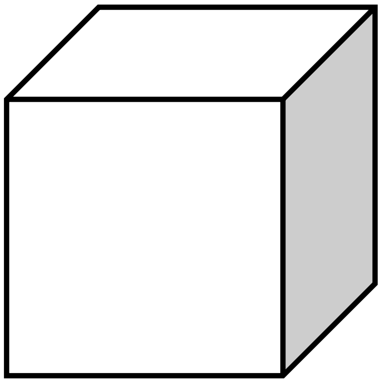


Body-Centered Cubic



Face-Centered Cubic

General Approach



$$\rho = \frac{mass\ (of\ unit\ cell)}{volume\ (of\ unit\ cell)}$$

$$\boldsymbol{mass\ of\ unit\ cell} = (number\ of\ atoms\ in\ unit\ cell\ * mass\ of\ each\ atom)$$

$$mass\ of\ atom = \frac{Molar\ Mass}{Avogadro's\ Number}$$

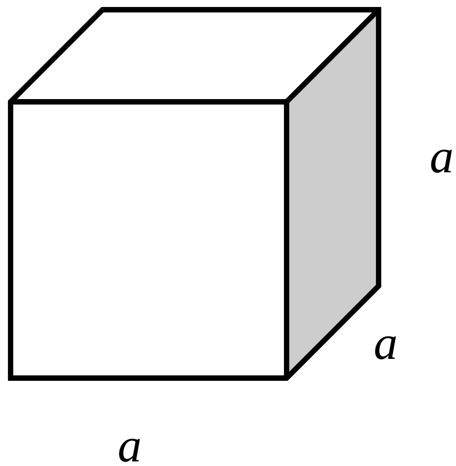
$$number\ of\ atoms\ in\ unit\ cell$$
$$= depends\ on\ structure\ (BCC, FCC, etc)$$

$$\boldsymbol{volume\ of\ unit\ cell} = f(arrangement\ and\ size\ of\ the\ atoms)$$

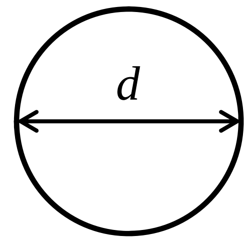
$$size\ of\ atom = collision\ diameter, or\ closest\ interatomic\ distance$$

Symbols

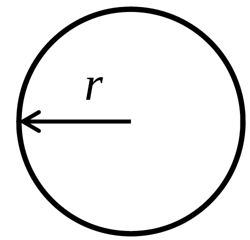
Unit Cell



Atom



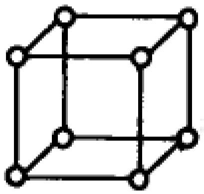
Atom



$$m = \frac{M}{N_A}$$

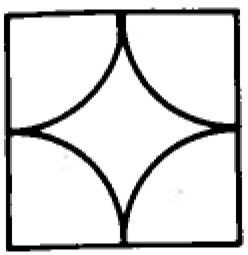
M = *Molar Mass*
m = *mass of one atom*
n = *number of atoms in unit cell*
r = *atomic radius*
d = *atomic diameter*
a = *length of side of unit cell*

$$\rho = \frac{mass\ (of\ unit\ cell)}{volume\ (of\ unit\ cell)}$$ = density of solid



SIMPLE

Simple Cubic - Density



$a = 2r = d$

SIMPLE CUBIC

n=1, NUMBER OF ATOMS IN THE UNIT CELL

VOLUME = d^3

DENSITY = $\frac{m}{d^3}$

$$m = \frac{M}{N_A}$$

- Mass of Unit Cell
- Number of atoms in unit cell

  = 1/8 x 8 corners = 1
- Mass = n*m = 1m

- Volume of Unit Cell
- Length of side of unit cell

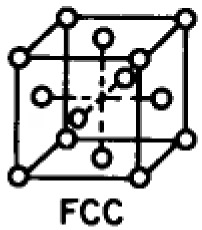
  = a = d
- Volume of unit cell

  = a^3 = d^3

$$\rho = \frac{mass\ (of\ unit\ cell)}{volume\ (of\ unit\ cell)} = \frac{m}{d^3}$$

m = mass of one atom

d = atomic diameter

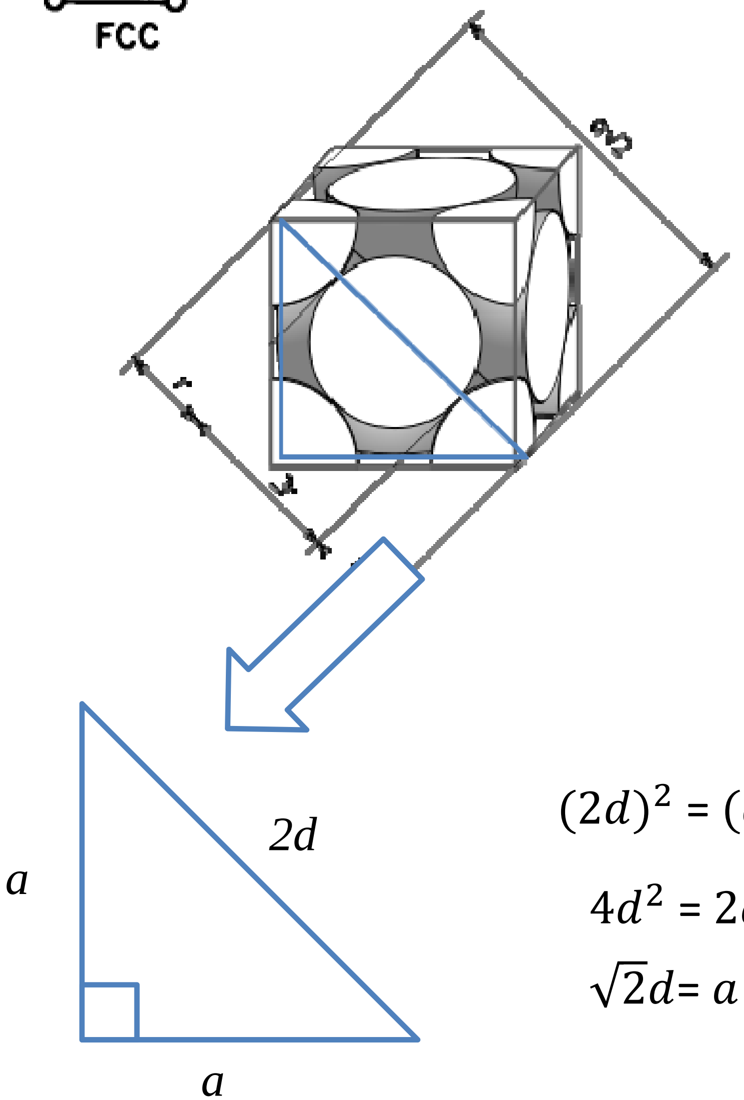


FCC - Density

- <u>Volume of Unit Cell</u>
- Length of side of unit cell

  = a = $\sqrt{2}d$
- Volume of unit cell

  = a^3 = $2\sqrt{2}d^3$

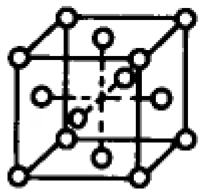


$(2d)^2 = (a)^2 + (a)^2$

$4d^2 = 2a^2$

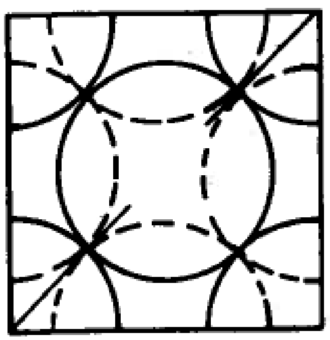
$\sqrt{2}d = a$

http://commons.wikimedia.org/wiki/File:Geometrie_cubique_faces_centrees.svg



FCC

FCC - Density



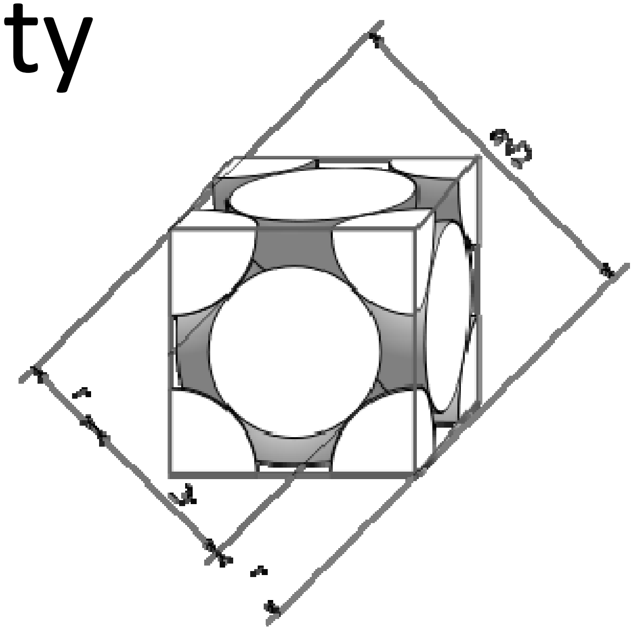
$a = \sqrt{2}\,d$

FCC (FACE - CENTERED CUBIC)

$n = 4$

$\text{VOLUME} = 2\sqrt{2}\,d^3$

$\text{DENSITY} = \frac{\sqrt{2}\,m}{d^3} = 1.414\,\frac{m}{d^3}$



- Mass of Unit Cell
- Number of atoms in unit cell

  = (1/8 x 8 corners) + (1/2 x 6 sides) = 4
- Mass = n*m = 4m

HCP Density the same as FCC

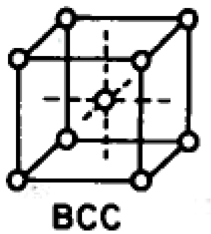
$$\rho = \frac{mass\ (of\ unit\ cell)}{volume\ (of\ unit\ cell)} = \frac{4m}{2\sqrt{2}d^3}$$

$$\rho = \frac{mass\ (of\ unit\ cell)}{volume\ (of\ unit\ cell)} = 1.414\,\frac{m}{d^3}$$

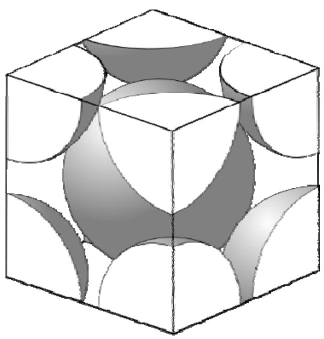
m = mass of one atom

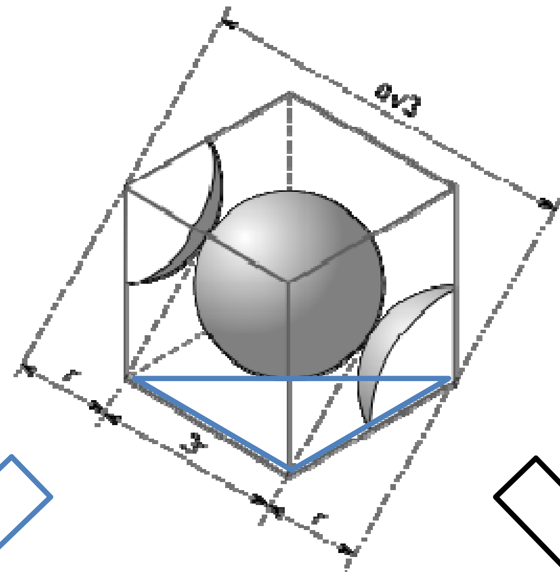
d = atomic diameter

http://commons.wikimedia.org/wiki/File:Geometrie_cubique_faces_centrees.svg



BCC - Density

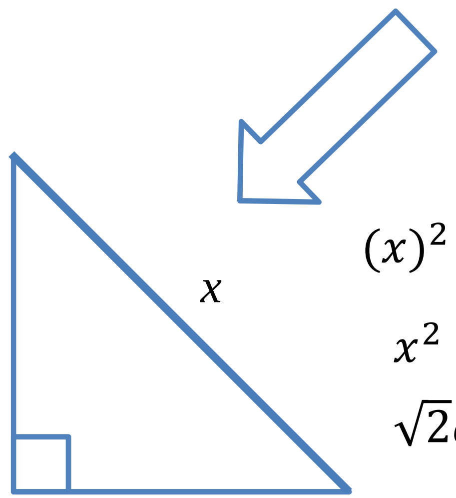




- Volume of Unit Cell
- Length of side of unit cell

  $= a \;\; = \frac{2}{\sqrt{3}} d$
- Volume of unit cell

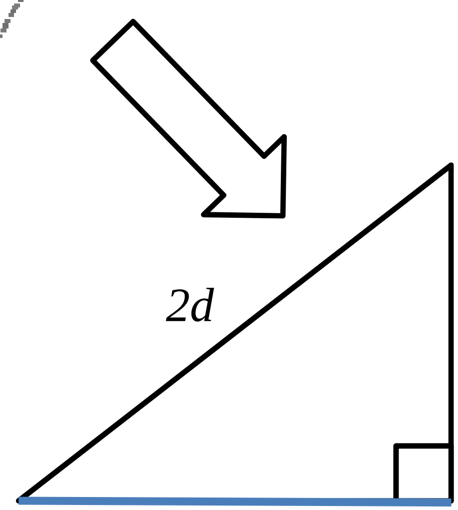
  $= a^3 \;\; = \frac{8}{3\sqrt{3}} d^3$



$$(x)^2 = (a)^2 + (a)^2$$

$$x^2 = 2a^2$$

$$\sqrt{2}a = x$$



$$(2d)^2 = (x)^2 + (a)^2$$

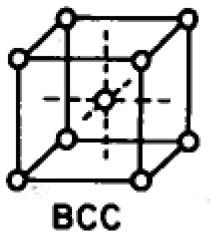
$$4d^2 = 2a^2 + a^2$$

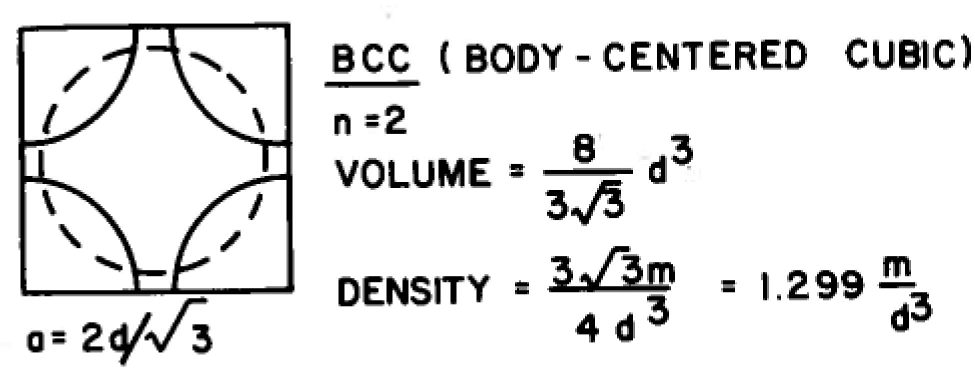
$$4d^2 = 3a^2$$

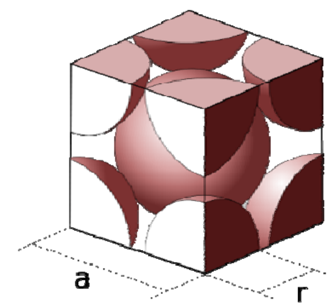
$$a = \frac{2}{\sqrt{3}} d$$

http://commons.wikimedia.org/wiki/File:Cubique_centre_atomes_par_maille.svg http://commons.wikimedia.org/wiki/File:Geometrie_cubique_centre.svg

BCC - Density







http://en.wikipedia.org/wiki/Atomic_packing_factor

- Mass of Unit Cell
- Number of atoms in unit cell

  = (1/8 x 8 corners) + (1 middle) = 2
- Mass = n*m = 2m

$$\rho = \frac{mass\ (of\ unit\ cell)}{volume\ (of\ unit\ cell)} = \frac{2m}{\frac{8}{3\sqrt{3}}d^3}$$

$$\rho = \frac{mass\ (of\ unit\ cell)}{volume\ (of\ unit\ cell)} = 1.299\,\frac{m}{d^3}$$

m = mass of one atom
d = atomic diameter

http://www.oocities.org/tokyo/fuji/1159/index3/mems.html

Relationship Between Variables

Density

- ρ

Substance / Mass

- m (from M)

Size of Atom / Volume

- σ (or d)

Structure

- Formula for Density

$$\rho = \frac{mass\ (of\ unit\ cell)}{volume\ (of\ unit\ cell)} = X\frac{m}{d^3}$$

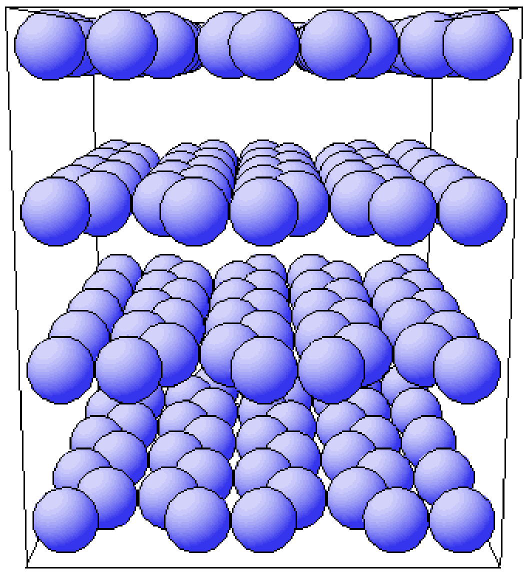
Void Fraction

- Unit cell has atoms + empty space
- Void fraction = fraction of unit cell that is empty space
- General formula:

$$Void\ Fraction = \frac{volume\ of\ unit\ cell\ - volume\ of\ atoms}{volume\ of\ unit\ cell}$$

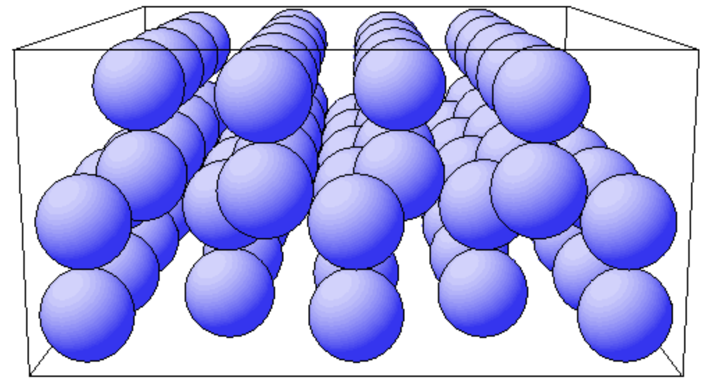
- Remember: atoms are spheres ($4/3\pi(d/2)^3$)

Graphite vs. Diamond



(0 0 1) Graphite (C)

vs.

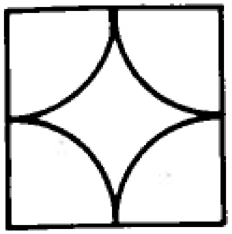


(1 1 1)c Diamond (C)

- Both graphite and diamond are C
- Arrangement of atoms can greatly influence properties (not just density)

http://www.cmmp.ucl.ac.uk/~ijf/3c25/surfex.html

Summary



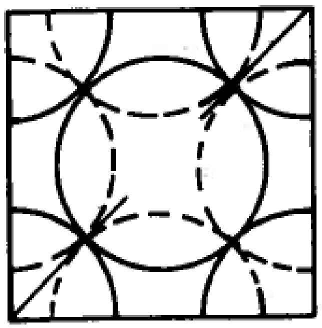
$a = 2r = d$

SIMPLE CUBIC

$n = 1$, NUMBER OF ATOMS IN THE UNIT CELL

VOLUME $= d^3$

DENSITY $= \frac{m}{d^3}$



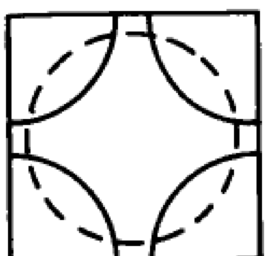
$a = \sqrt{2}\,d$

FCC (FACE - CENTERED CUBIC)

$n = 4$

VOLUME $= 2\sqrt{2}\,d^3$

DENSITY $= \frac{\sqrt{2}\,m}{d^3} = 1.414\,\frac{m}{d^3}$



$a = 2d/\sqrt{3}$

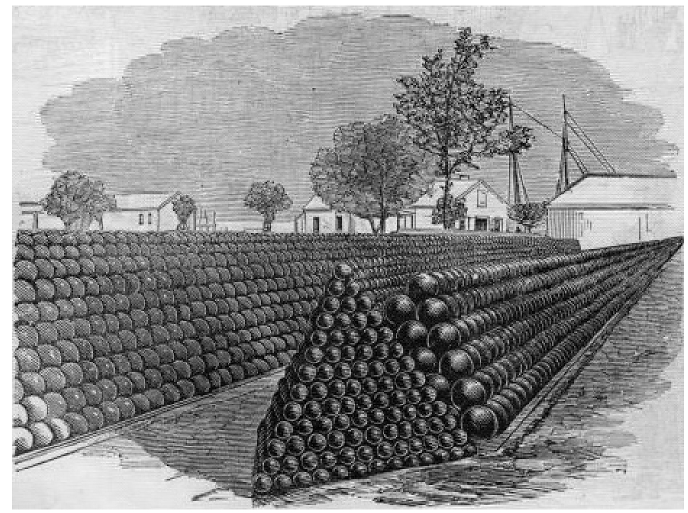
BCC (BODY - CENTERED CUBIC)

$n = 2$

VOLUME $= \frac{8}{3\sqrt{3}}\,d^3$

DENSITY $= \frac{3\sqrt{3}\,m}{4\,d^3} = 1.299\,\frac{m}{d^3}$

?



Harpers Weeksly, June 29, 1861 - page 401