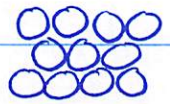
1/28/2019

Chapter 12: Solids + Modern Materials.

12.1 Graphene

12.2 X-Ray diffraction.

12.3 Unit Cells + Basic Structure

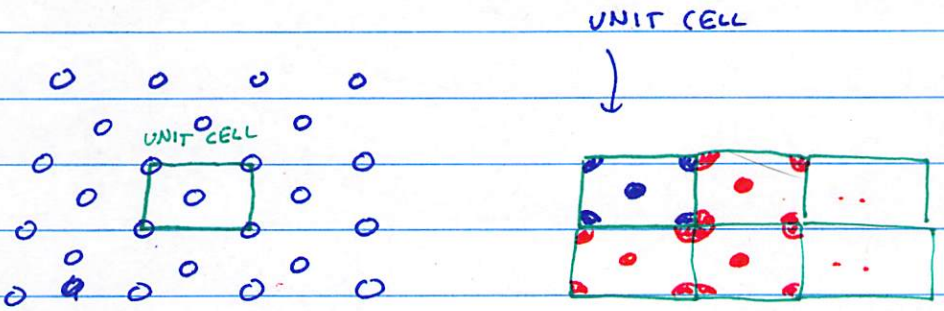
Many solids are crystalline (ordered)  , but some are amorphous  (like a frozen liquid)

$Fe(s)$, $H_2O(s)$

glass, tar

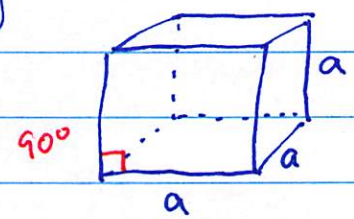
- crystalline solids have a repeating pattern ~ UNIT CELL

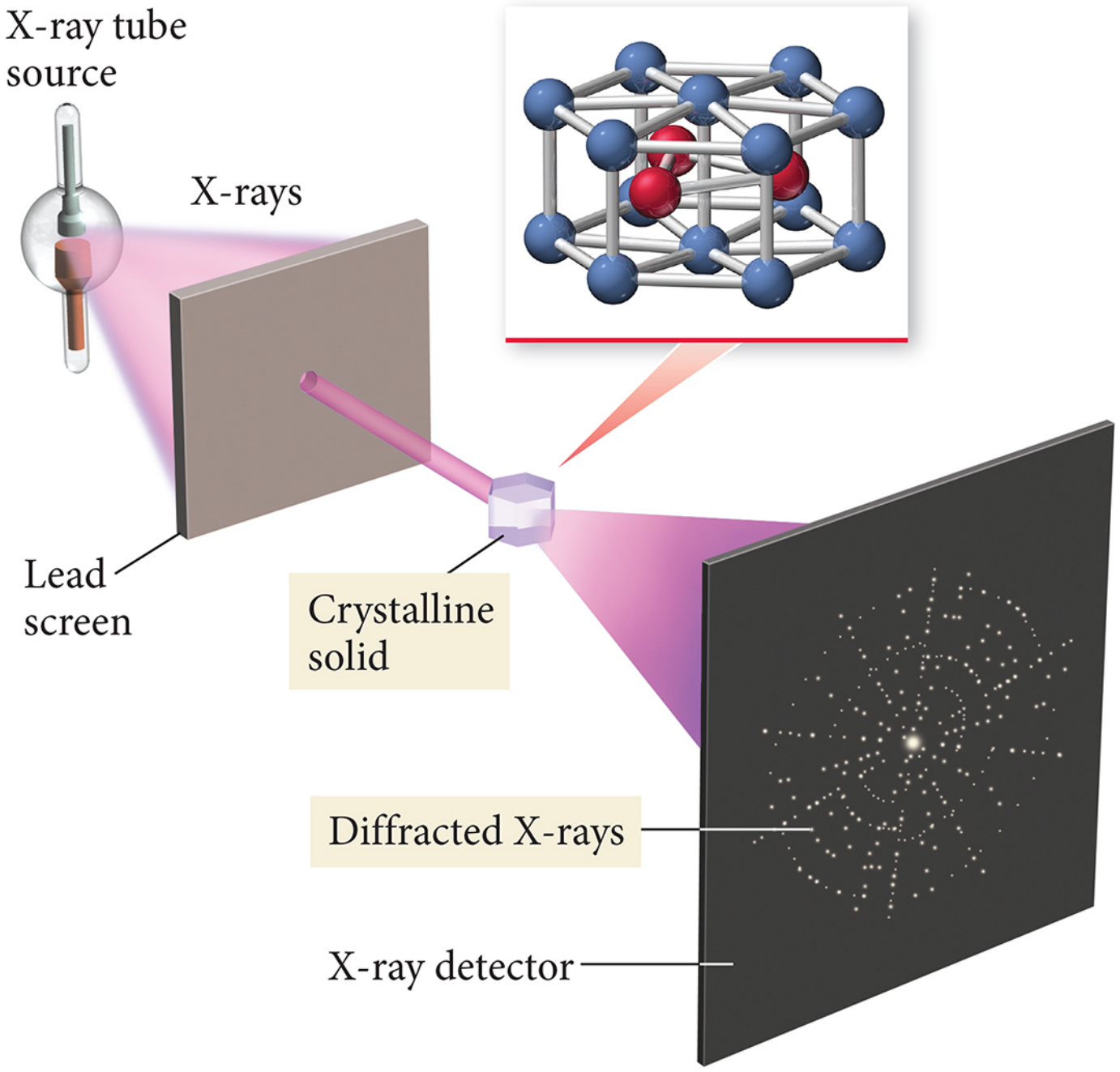
- can "stamp out" structure from this building block

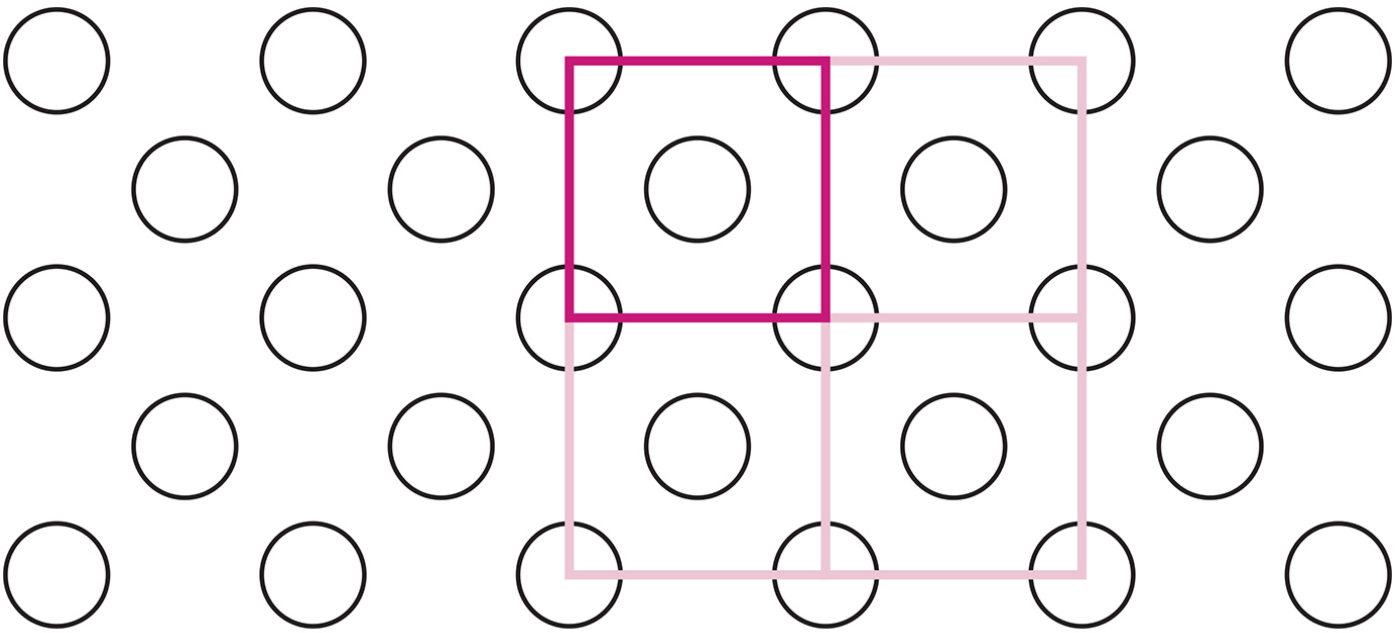


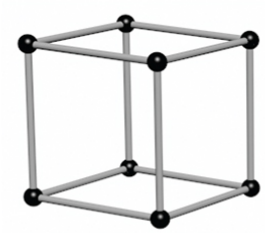
In 3-D, there are only 7 basic shapes for our unit cells

We'll only look @ CUBES in 1142E









Cubic

$a = b = c$

$\alpha = \beta = \gamma = 90°$

Tetragonal

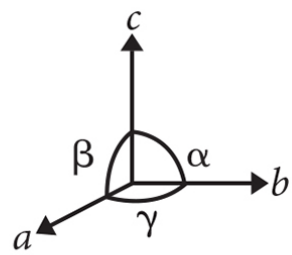
$a = b \neq c$

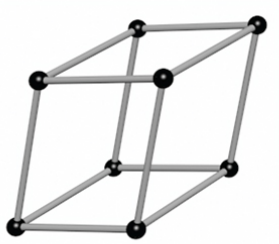
$\alpha = \beta = \gamma = 90°$

Orthorhombic

$a \neq b \neq c$

$\alpha = \beta = \gamma = 90°$





Rhombohedral

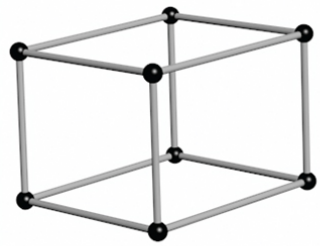
$a = b = c$

$\alpha = \beta = \gamma \neq 90°$

Hexagonal

$a = b \neq c$

$\alpha = \beta = 90°, \gamma = 120°$



Monoclinic

$a \neq b \neq c$

$\alpha = \beta = 90°, \gamma \neq 90°$

Triclinic

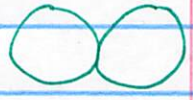
$a \neq b \neq c$

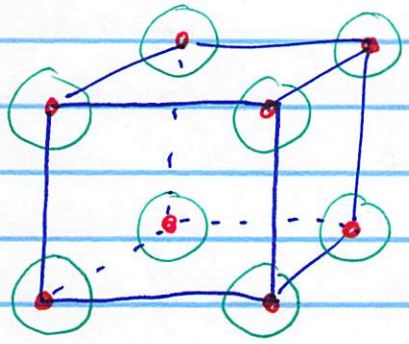
$\alpha \neq \beta \neq \gamma$

There are 3-kinds of CUBIC unit cells

(1) Simple cubic (unit cell)

reality:





• = lattice point

- can hang atoms/ions/... on each lattice point

(52% packing efficiency)

How many atoms are inside this cell?

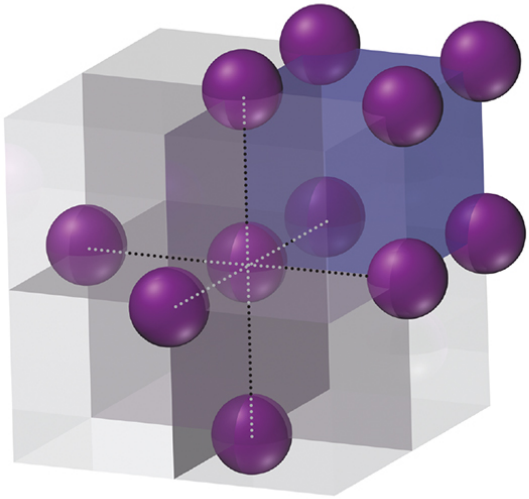
$= 8 \times \frac{1}{8} = 1$

↳ fraction inside

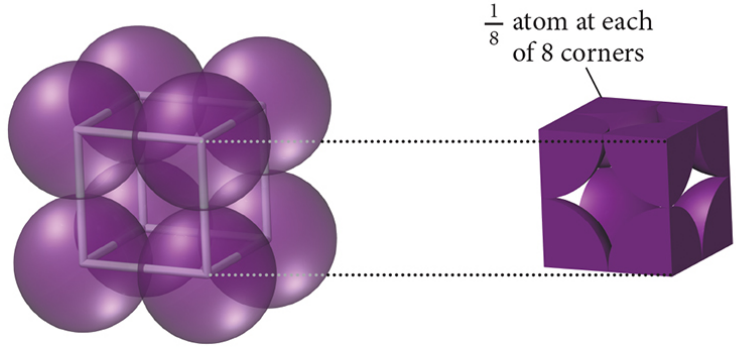
ex: Po(s)

Simple Cubic Unit Cell

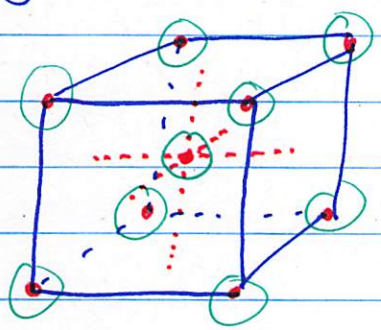
Coordination number = 6



Atoms per unit cell = $\frac{1}{8} \times 8 = 1$



2) Body Centered Cubic (bcc)



corner / body

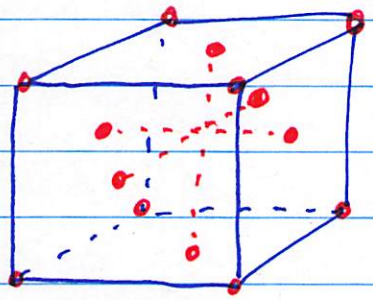
$\#\text{atoms/cell} = 8 \times \left(\frac{1}{8}\right) + 1 \times (1) = 2$

ex: Ba(s)
Fe(s)

68% packing efficiency

3) Face-centered cubic (fcc) / cubic closest pack (ccp)

74% efficient

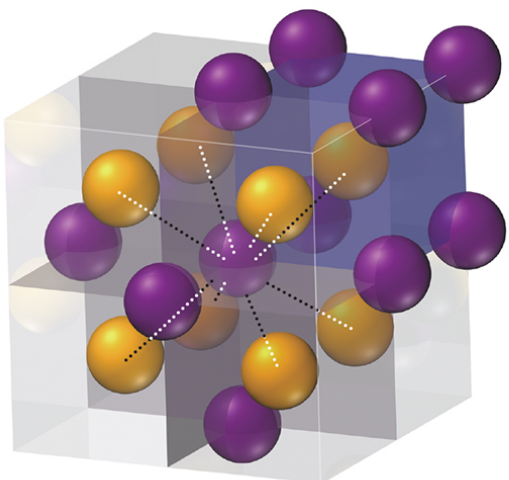


corner / face

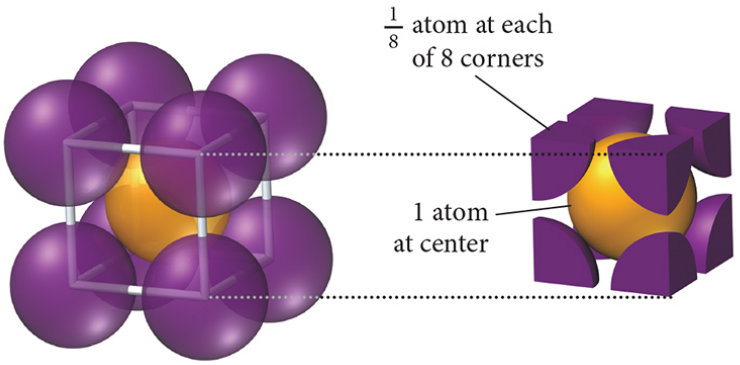
$\#\text{atoms/cell} = 8 \times \left(\frac{1}{8}\right) + 6 \times \left(\frac{1}{2}\right) = 4$

Body-Centered Cubic Unit Cell

Coordination number = 8



Atoms per unit cell = $\left(\frac{1}{8} \times 8\right) + 1 = 2$



Face-Centered Cubic Unit Cell

Coordination number = 12

Atoms/unit $= \left(\frac{1}{8} \times 8\right) + \left(\frac{1}{2} \times 6\right) = 4$