PHY 555 Lecture 3

Crystal Structures

•Bravais lattice: simply describes the periodic arrangement of the repeated units of a crystal;
•Crystal: any structure that is made up from a well defined unit structure infinitely repeated following a fixed geometrical rule (periodicity).
•Crystal structure: periodic[a], infinite repetition[b] of identical structural units[c].

a. Translational symmetry:

Def. Bravais Lattice= all points defined by

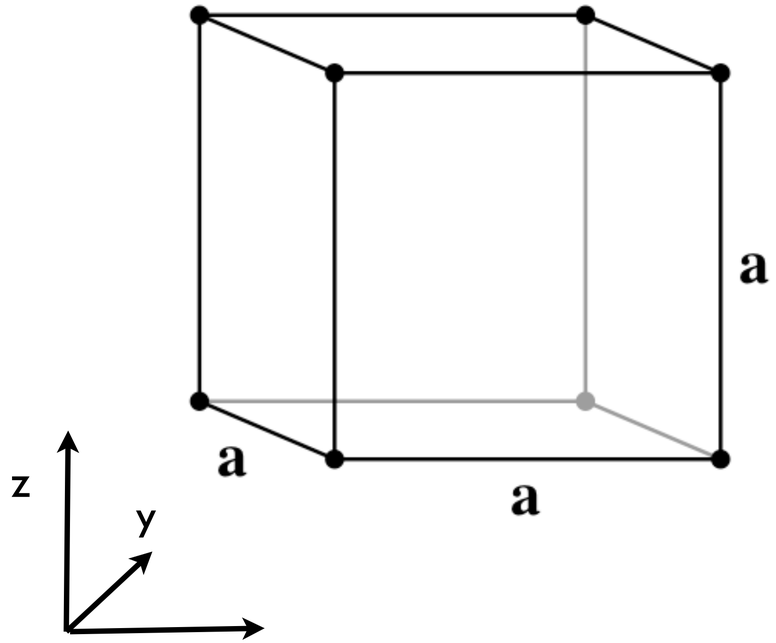
$$\vec{R} \quad (\mathrm{latticevector}) = n\vec{a}_1 + n\vec{a}_2 + n\vec{a}_3; \qquad \mathrm{n}_1, \mathrm{n}_2, \mathrm{n}_3 \mathrm{integers}$$

$\hat{a}_{1,2,3}$= primitive lattice vectors (non coplanar)⇒generate the lattice

b. N~10^{23} ~∞⇒ Bulk properties are independent of surfaces

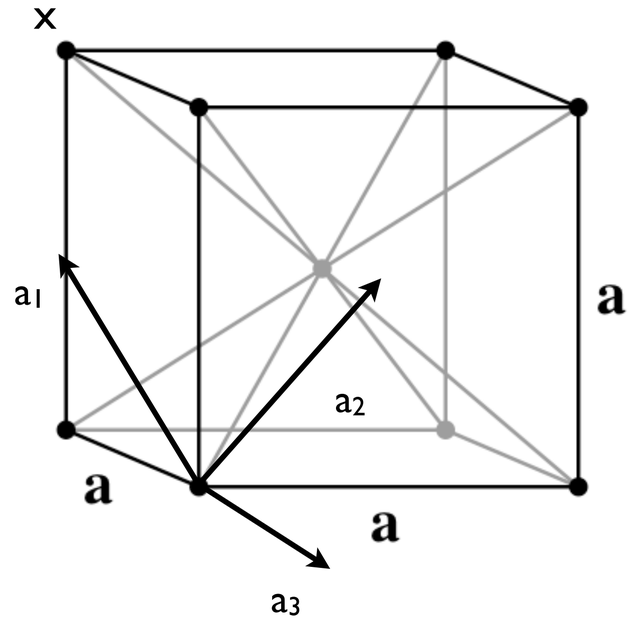
c. Structural units associated to each lattice point≡ basis = atom (or collection of atoms) or molecules.

Summary: Crystal structure = Bravais lattice + basis



Simple Cubic: SC

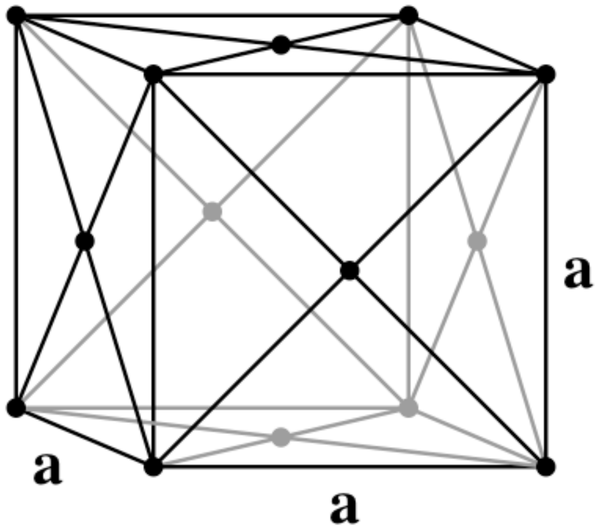
$$\vec{a_1} = a\vec{i}$$
$$\vec{a_2} = a\vec{j}$$
$$\vec{a_3} = a\vec{k}$$



Body Centered Cubic: BCC

$$\vec{a_1} = a\vec{i} \qquad \vec{a_1} = a/2(-\vec{i} + \vec{j} + \vec{k})$$
$$\vec{a_2} = a\vec{j} \qquad \vec{a_2} = a/2(\vec{i} - \vec{j} + \vec{k})$$
$$\vec{a_3} = a/2(\vec{i} + \vec{j} + \vec{k}) \qquad \vec{a_3} = a/2(\vec{i} + \vec{j} - \vec{k})$$

Note: images from wikipedia, http://en.wikipedia.org/wiki/Cubic_crystal_system

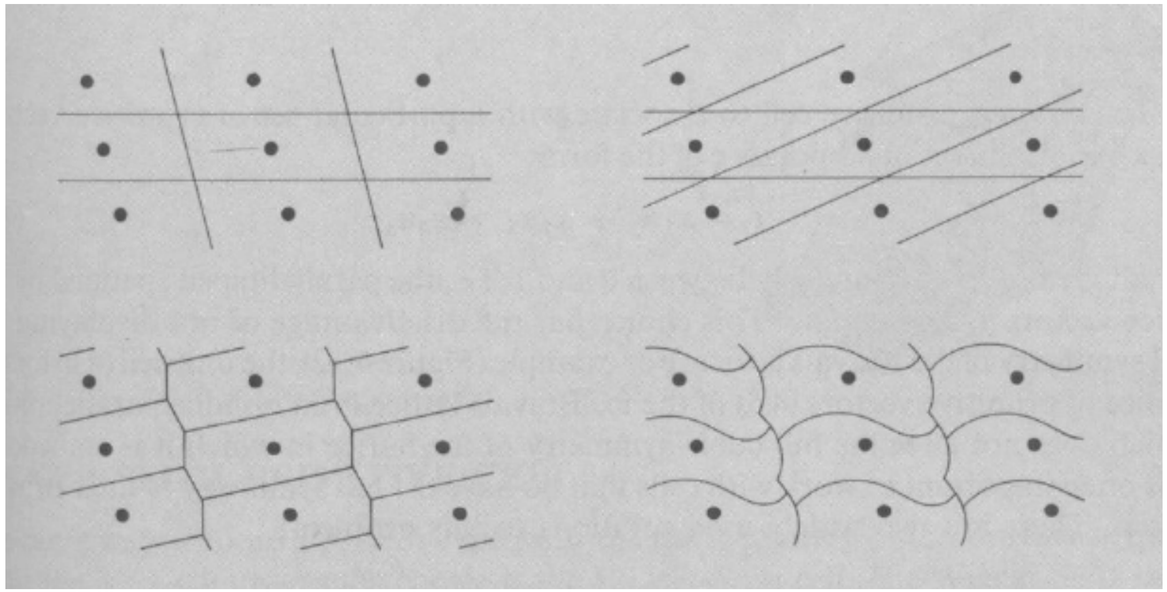


Face Centered Cubic: FCC

$$\vec{a_1} = a/2(\vec{j} + \vec{k})$$
$$\vec{a_2} = a/2(\vec{i} + \vec{k})$$
$$\vec{a_3} = a/2(\vec{i} + \vec{j})$$

Primitive Unit Cell

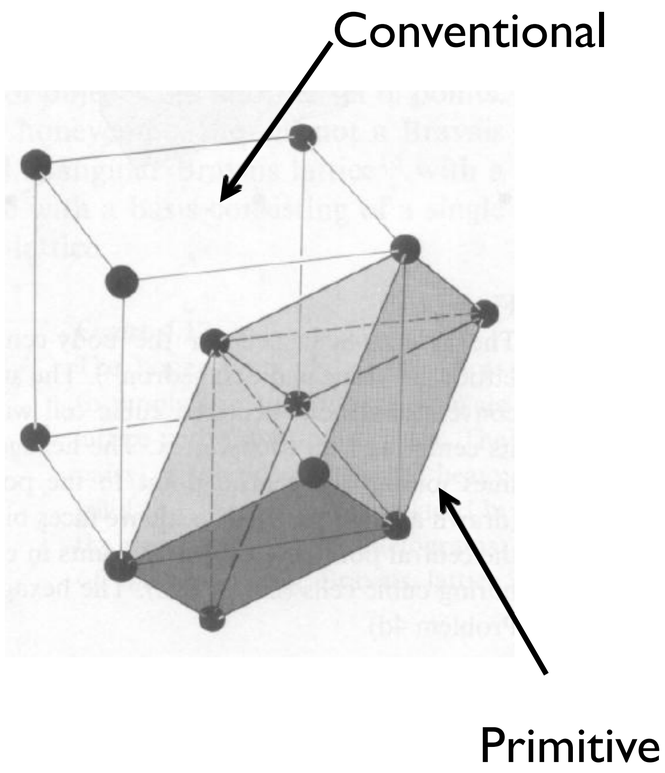
The Space-filling Volume (or hyper-volume) per lattice point can take any arbitrary shape. Whichever volume that when translated though **ALL** vectors in a Bravais lattice fills the full space (no overlapping) represents a primitive unit cell.



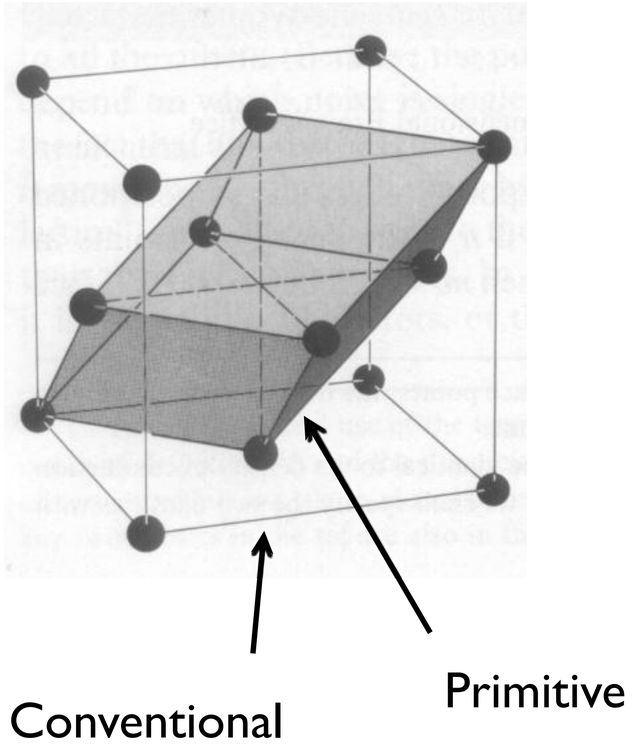
Conventional unit cell

Whichever volume that when translated though a **SUBSET** of vectors in a Bravais lattice vectors fills the full space (no overlapping) represents a primitive unit cell.

bcc

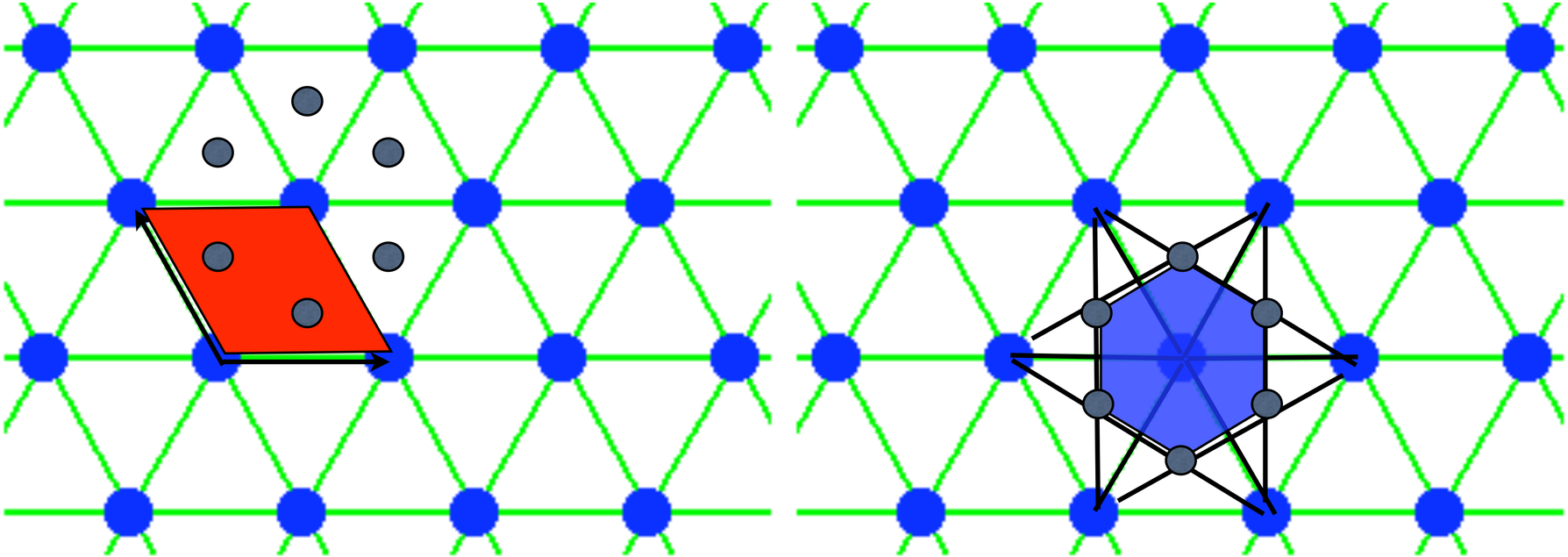


fcc



Unit Cell

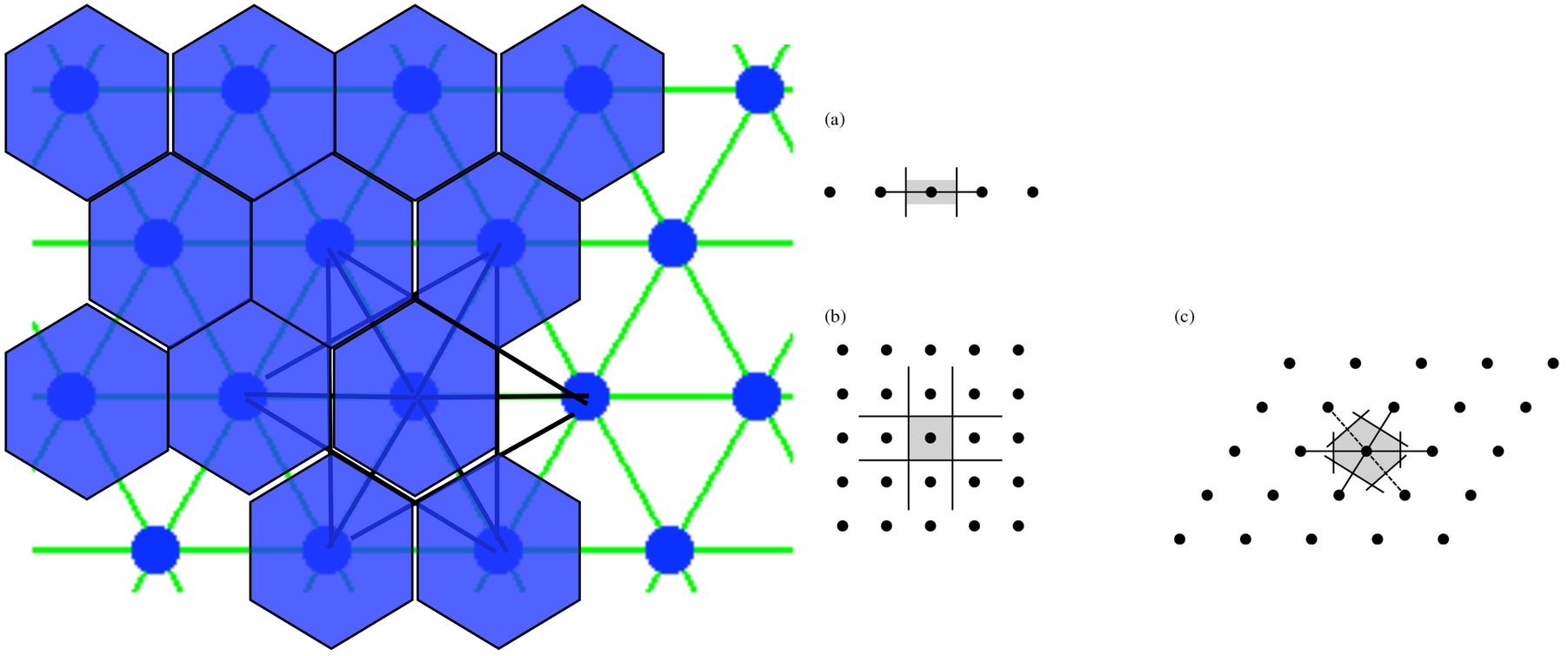
Bravais Lattice (NOT crystal) of graphene: Hexagonal cell



http://home.hetnet.nl/~turing/complete_hex_motif_2a.gif

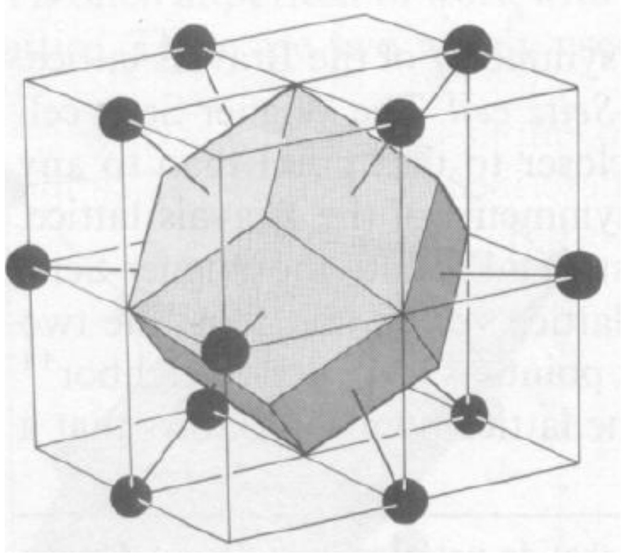
Wigner-Seitz Unit cell

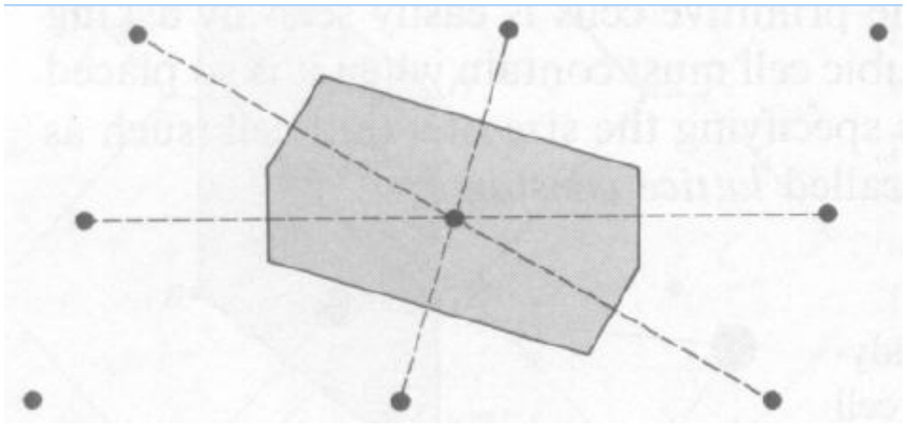
Reflects all (point) symmetries of the Bravais lattice itself.

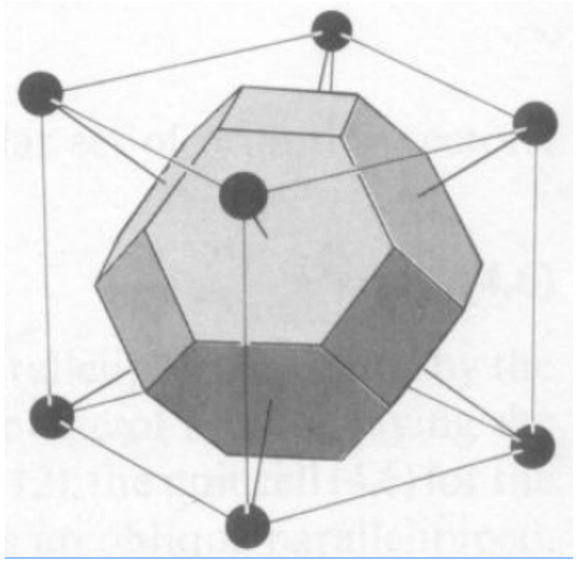


Wigner-Seitz Unit cell

- Region of the space closer to a given lattice point than to any other latt. point.
- Draw Lines from the origin to all nearby lattice points
- Volume enclosed by perpendicular bisector planes
- Shows full Bravais lattice point symmetry

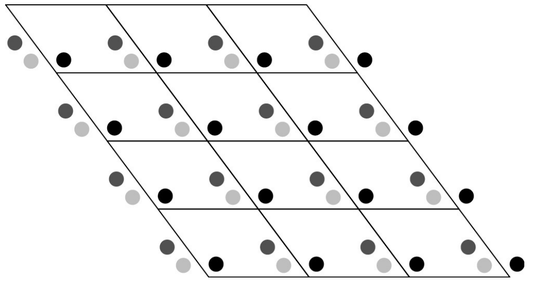




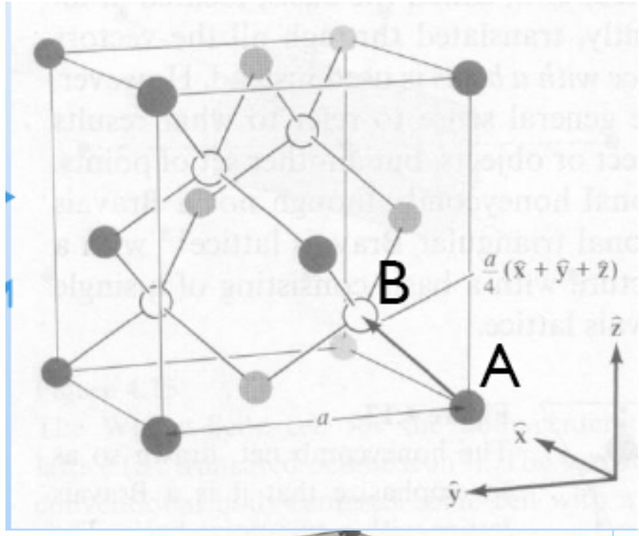


Ashcroft & Merming, Ch 4.

Crystal= Bravais Lattice +Basis



Diamond Structure: Two fcc lattices displaced along body diagonal: fcc+ {0, a/4(x+y+z)}



- Diamond Structure

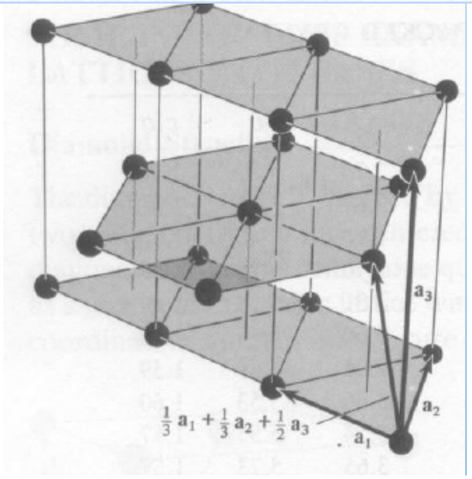
(fcc + 2 identical atom basis; A=B)

- Zinc-Blend Structure

(fcc + 2 different atom basis; A≠B)

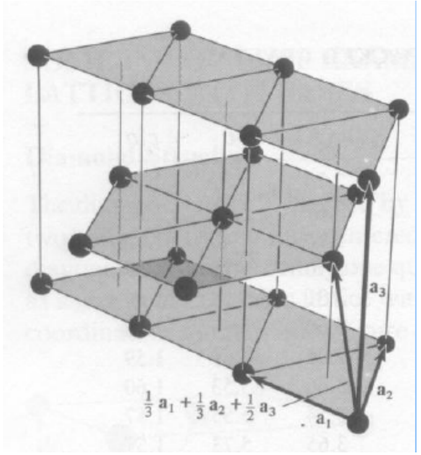
- Hexagonal Close Packed Structure (hcp)

(hexagonal lattice + 2 identical atom basis)

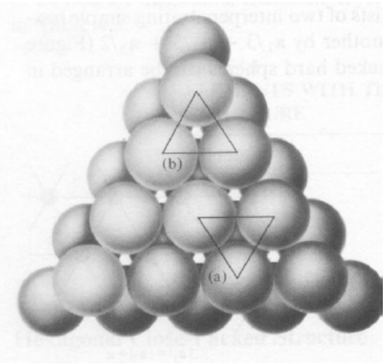


Close-Packed Structures

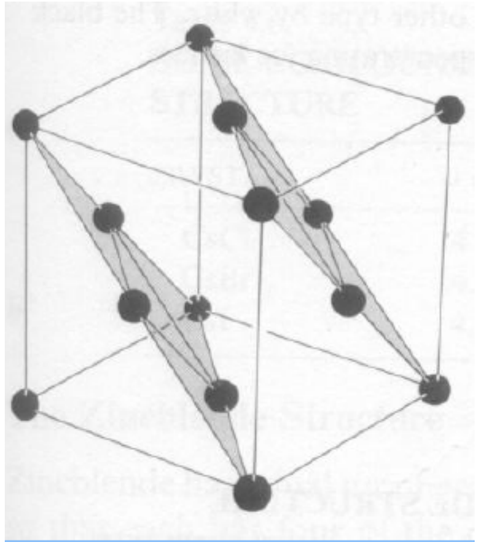
hcp



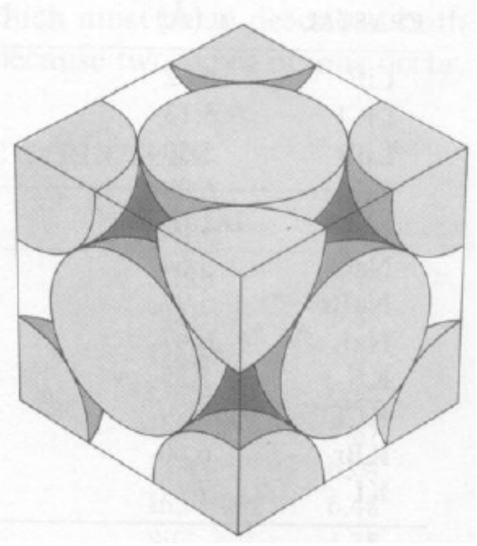
AB-AB packing
of “marbles”



fcc



ABC-ABC packing
of “marbles”



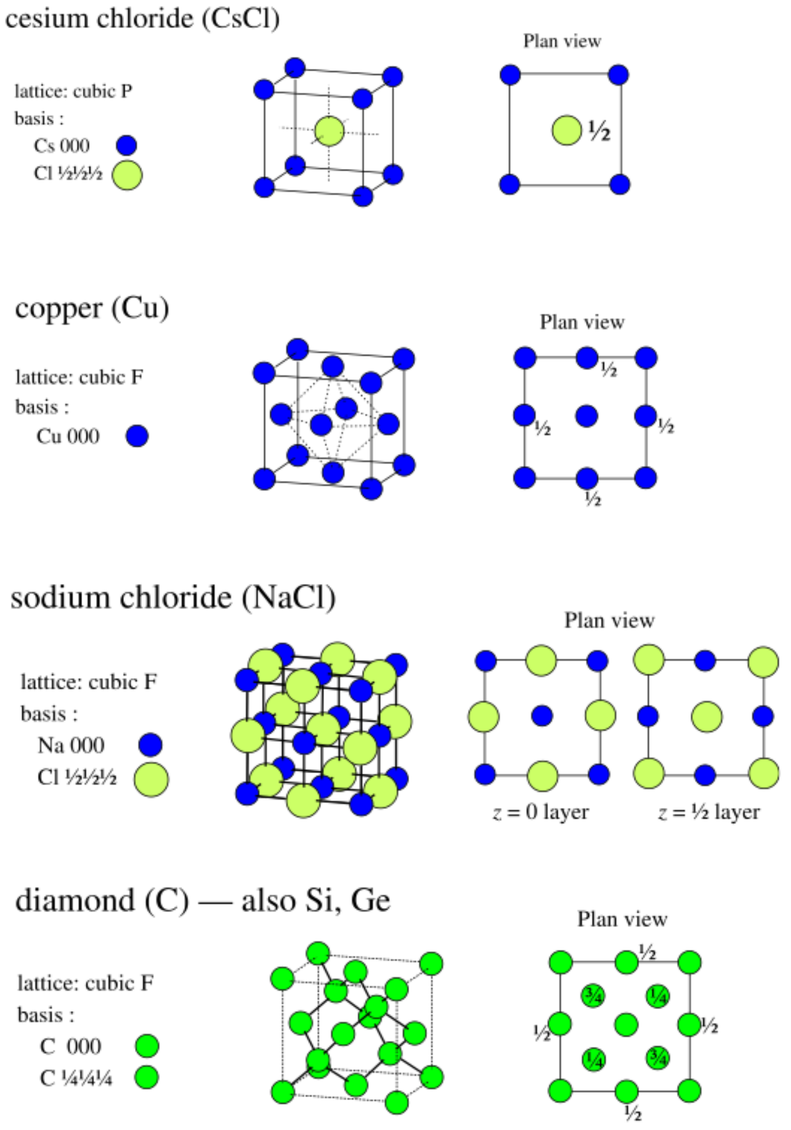


Figure 11.16: Some examples of real crystals with simple structures. Note that in all cases the basis is described with respect to the primitive unit cell of a simple cubic lattice.

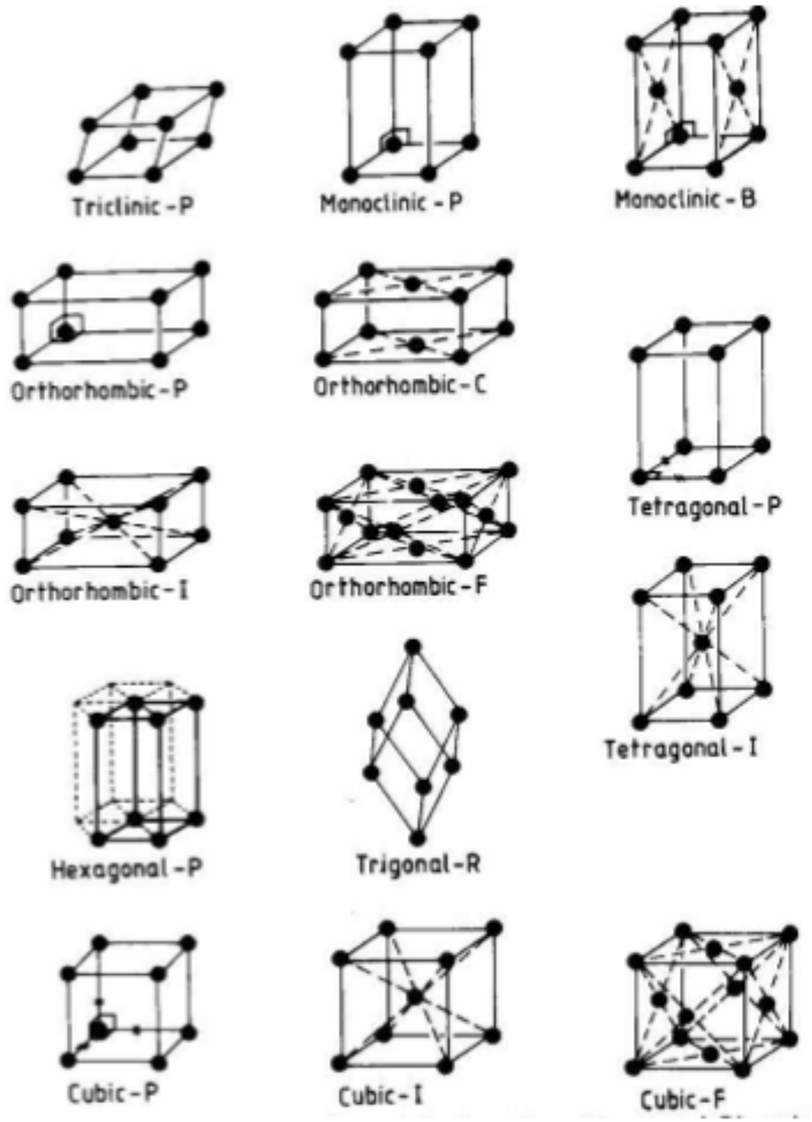
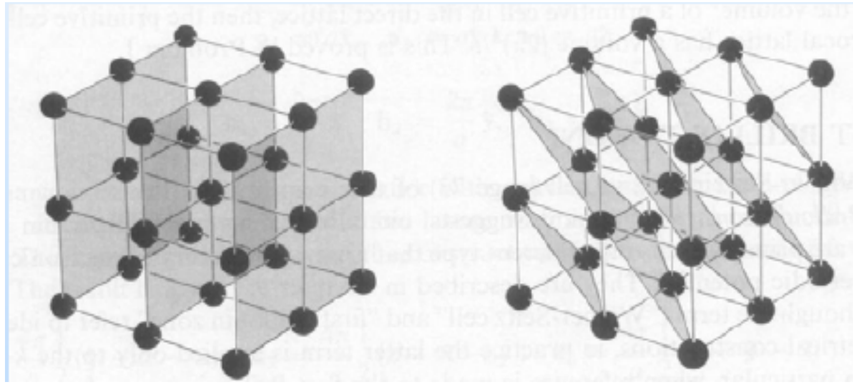


Figure 11.15: Unit cells for All of the Three Dimensional Bravais Lattice Types.

- V = volume of unit cell
- V* = volume of reciprocal unit cell
- $V\,V^* = (2\pi)^d$ (d = dimension, 1, 2, 3)
- Reciprocal of fcc is bcc and vice versa
- Reciprocal of hexagonal is hexagonal

[First] **Brillouin zone**≡Wigner Seitz Cell of the momentum (i.e. wave vector) space.

•Any plane containing at least three non-colinear Bravais Lattice points ≡Lattice Plane



•For a given BL and a LP, BL = family of LP

•Any family of lattice planes can be labeled by a reciprocal lattice vector K, which is perpendicular to the lattice planes. The minimum non-zero length of K is given by $2\pi/d$, where d is the spacing between lattice planes.

Any lattice plane is a 2d Bravais Lattice,
characterized by two vectors, which we can call
a1 and **a2**.

Now, choose any vector connecting
a lattice point of a given lattice plane and
another point of the next lattice plane.Call this **a3**.
a1,a2,a3 are primitive vectors.

Let **b1,b2,b3** be their reciprocal primitive vectors.
By construction, **b3** is perpendicular to our lattice
planes. This is because all 3 rlv are perpendicular to the 3 dlv.

Furthermore, $\mathbf{b3} \cdot \mathbf{a3} = 2\pi$.
Since d is the lattice plane separation, $\mathbf{b3} \cdot \mathbf{a3} = |\mathbf{b3}|d$, and thus
$|\mathbf{b3}| = 2\pi/d$. QED.

Miller Indices of a Lattice plane A

We know that families of lattice planes are associated to unique ∞ reciprocal vectors $\vec{K}$. Miller indeces of the plane are nothing else but the coordinates of the shortest reciprocal lattice vector perpendicular to a family of planes.

The coordinates of the miller planes are given in a basis of a specific set of primitive reciprocal vectors

a plane with miller indeces h, k, l is $\perp$ to the reciprocal vector $\vec{K} = h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3$

Say a plane $A \perp \vec{h} = \sum l_i \vec{b}_i$, l_i's no common factors

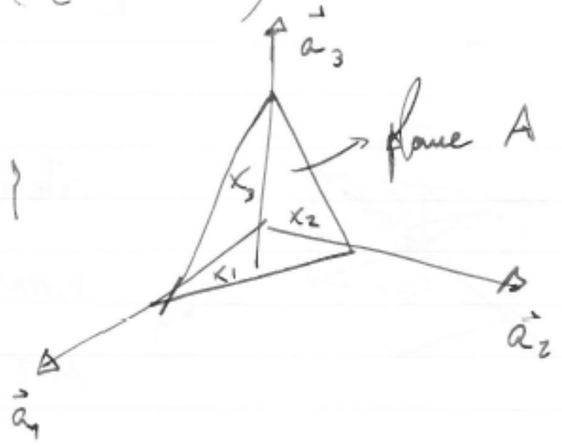
dist $A_N - A_{N+1} = 2\pi/k$

The miller indices for $A = (l_1, l_2, l_3)$

Geometrical meaning

A intercepts the axis $\{\vec{a}_i\}$

at $x_1, x_2 x_3$



The ec. for A :

$\vec{h} \cdot \vec{r} = cte$

$\vec{h}(x_1 \vec{a}_1) = \vec{h}(x_2 \vec{a}_2) = \vec{h}(x_3 \vec{a}_3) = 2\pi l_1 x_1 = 2\pi l_2 x_2 = 2\pi l_3 x_3$

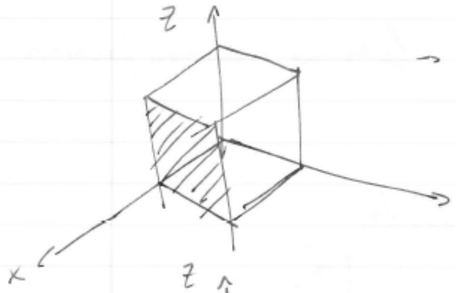
$l_1 x_1 = l_2 x_2 = l_3 x_3 = cte$

Miller indices $= (l_1, l_2, l_3) \propto \left(\frac{1}{x_1}, \frac{1}{x_2}, \frac{1}{x_3}\right)$

How To: Determine $x_1, x_2 x_3 \Rightarrow$ where plane intercepts the axis ; Take $\frac{1}{x_i}$; multiply by a common factor to obtain the smallest integers.

Conventions to specify directions

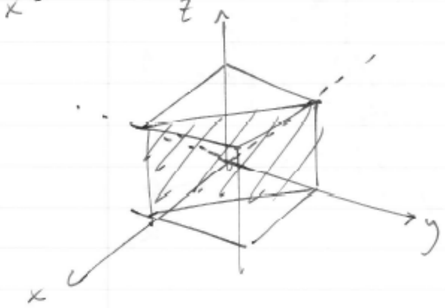
1.- Usually (for cubic lattices) they are defined with respect to the conventional unit cell



→ intercepts $(1, \infty, \infty)$

inverse $(1, 0, 0)$

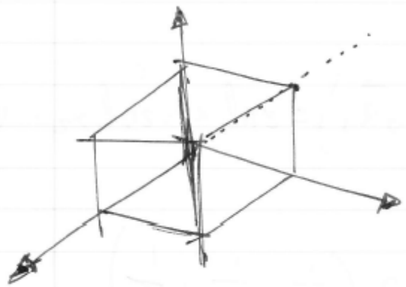
M.I (100)



intercepts $(1, 1, \infty)$

inverse $(1, 1, 0)$

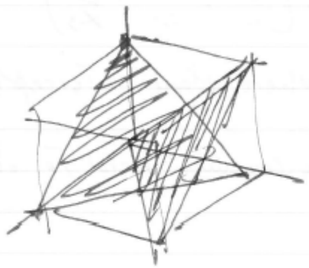
M.I (110)



intercepts $(0,0,0)$ => We need to take a parallel plane

$(1,-1,0)$ eq. → $(\bar{1},1,0)$

M.I $(1,\bar{1},0)$ $(\bar{1}\,1\,0)$



Intercepts $(1,1,1)$

M.I (111)

Notations :

(100) a lattice plane

$(0\,-1\,0) \equiv (0\,\bar{1}\,0)$

$\{100\} = (100), (\bar{1}00), (010)$ etc

$[100] \equiv$ direction along $\vec{a}_1$

$[xyz]$ direction along $x\vec{a}_1 + y\vec{a}_2 + z\vec{a}_3$

$\langle 100 \rangle \equiv [100], [\bar{1}00], [010]$ etc