Crystal Structures

Crystal = Lattice + Basis

Crystal = Lattice + Motif

Motif or basis:

an atom or a group of atoms associated with each lattice point

14 ***BRAVAIS LATTICES*** + 7 ***CRYSTAL SYSTEMS***

⇒ **Only 7 *different shapes of unit cell can be stacked together to completely fill all space without overlapping*.**

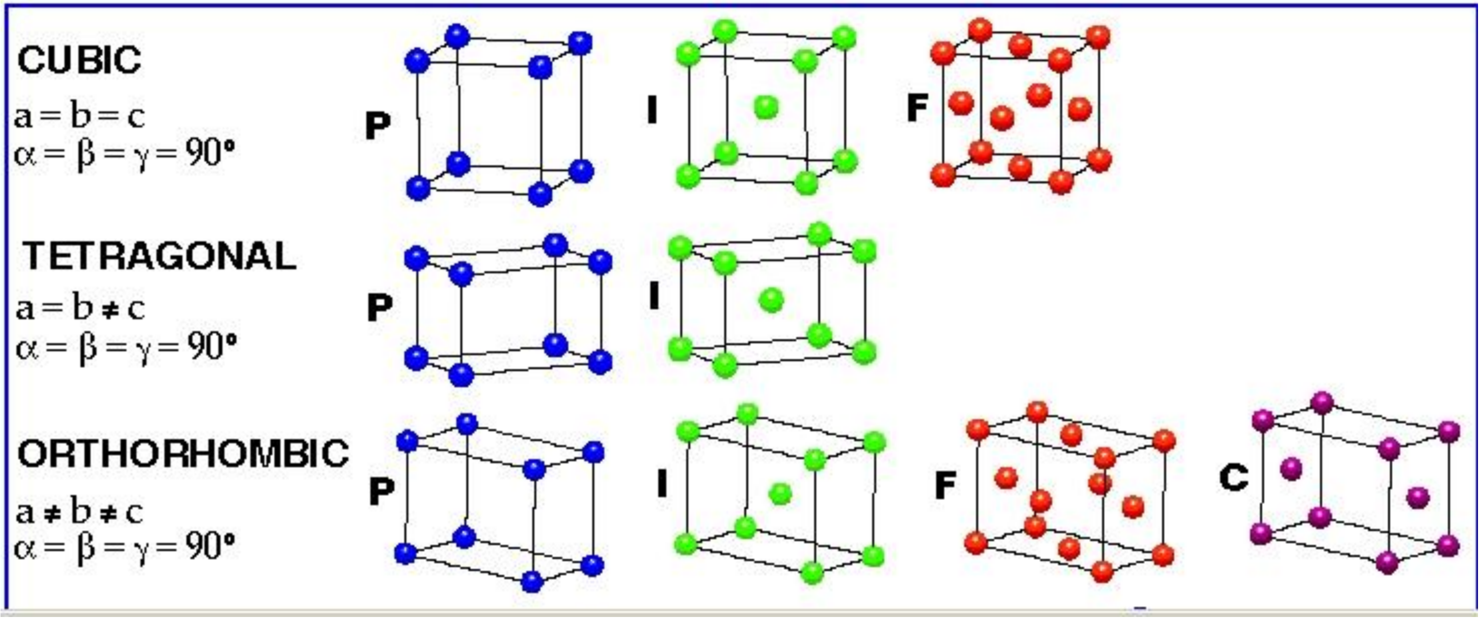
- This gives 7 crystal systems, into which all crystal structures can be classified. These systems & subsystems are:

1. **Cubic System** (SC, BCC, FCC)
2. **Hexagonal System** (S)
3. **Triclinic System** (S)
4. **Monoclinic System** (S, Base-C)
5. **Orthorhombic System** (S, Base-C, BC, FC)
6. **Tetragonal System** (S, BC)
7. **Trigonal** (**Rhombohedral**) **System** (S)

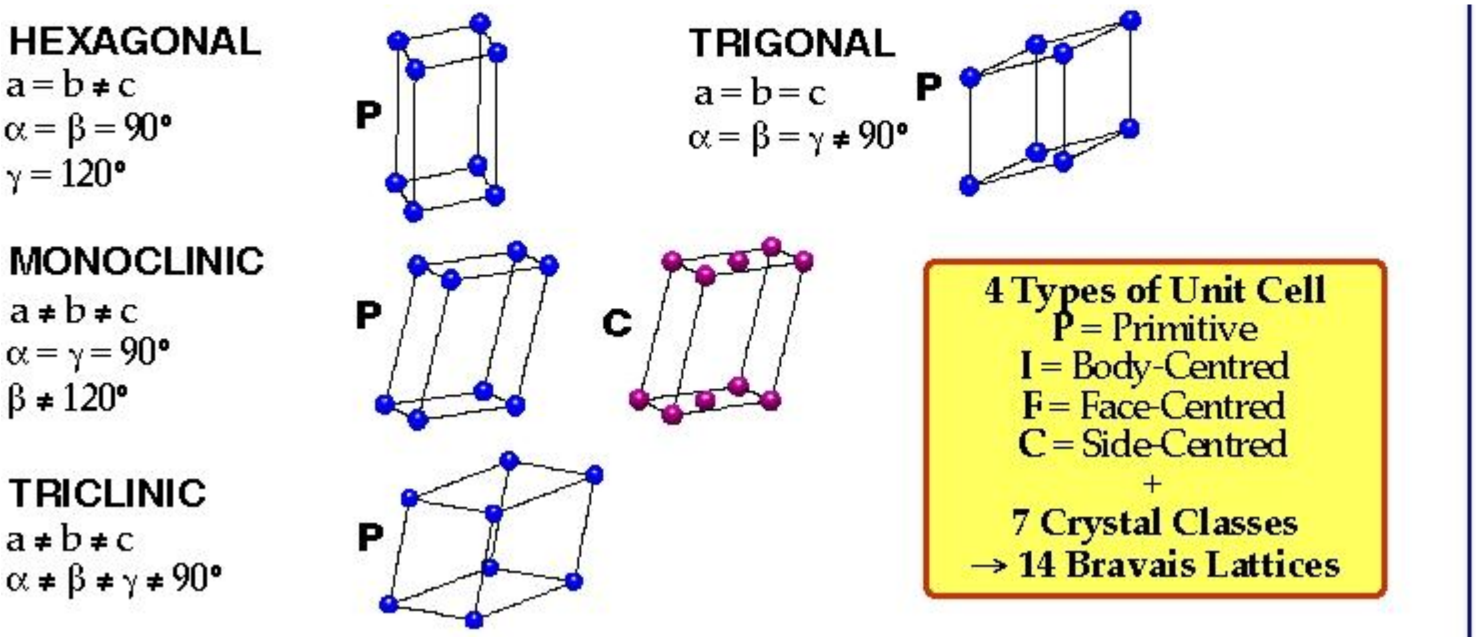
Summary: Fourteen Bravais Lattices in Three Dimensions

The 14 possible **BRAVAIS LATTICES**

{note that spheres in this picture represent lattice points, not atoms!}



Fourteen Bravais Lattices …



HEXAGONAL
$a = b \neq c$
$\alpha = \beta = 90°$
$\gamma = 120°$

TRIGONAL
$a = b = c$
$\alpha = \beta = \gamma \neq 90°$

MONOCLINIC
$a \neq b \neq c$
$\alpha = \gamma = 90°$
$\beta \neq 120°$

TRICLINIC
$a \neq b \neq c$
$\alpha \neq \beta \neq \gamma \neq 90°$

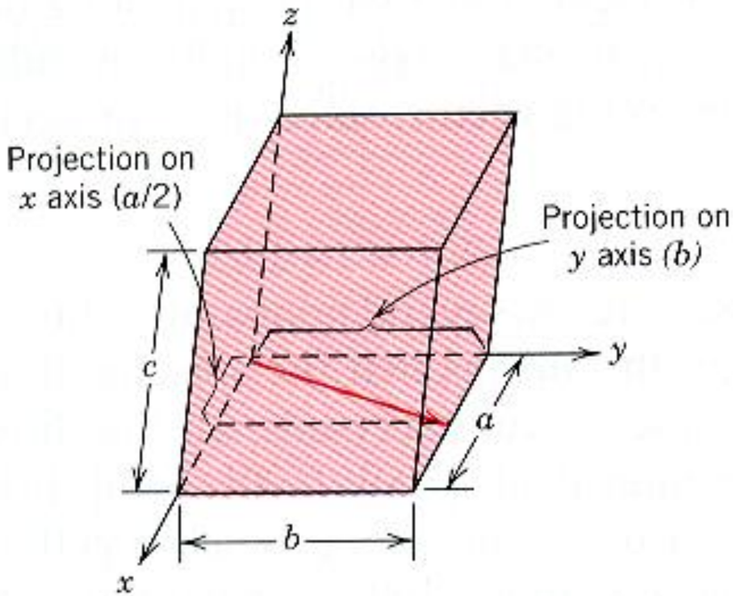
4 Types of Unit Cell
P = Primitive
I = Body-Centred
F = Face-Centred
C = Side-Centred
+
7 Crystal Classes
→ **14 Bravais Lattices**

Miller indices

A Miller index is a series of coprime integers that are inversely proportional to the intercepts of the crystal face or crystallographic planes with the edges of the unit cell.

It describes the orientation of a plane in the 3-D lattice with respect to the axes.

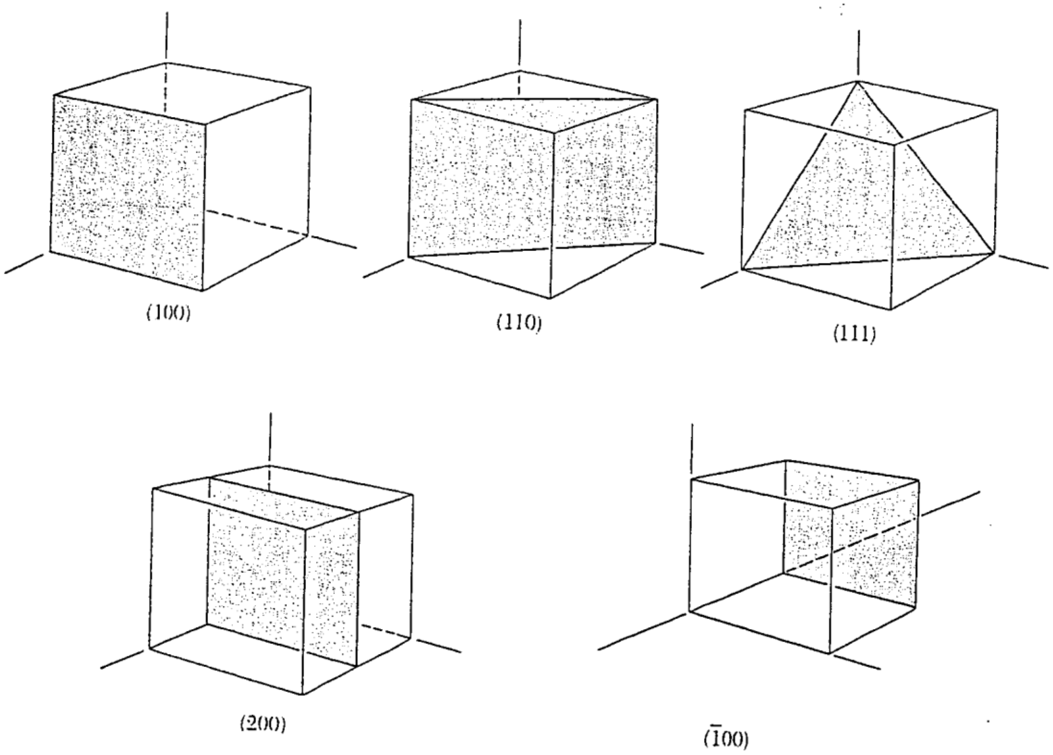
The general form of the Miller index is (h, k, l) where h, k, and l are integers related to the unit cell along the a, b, c crystal axes.



What is this ***Direction ?????***

	x	y	z
Projections:	a/2	b	0c
Projections in terms of a,b and c:	1/2	1	0
Reduction:	1	2	0
[brackets]		**[120]**	

Indices of Planes: Cubic Crystal

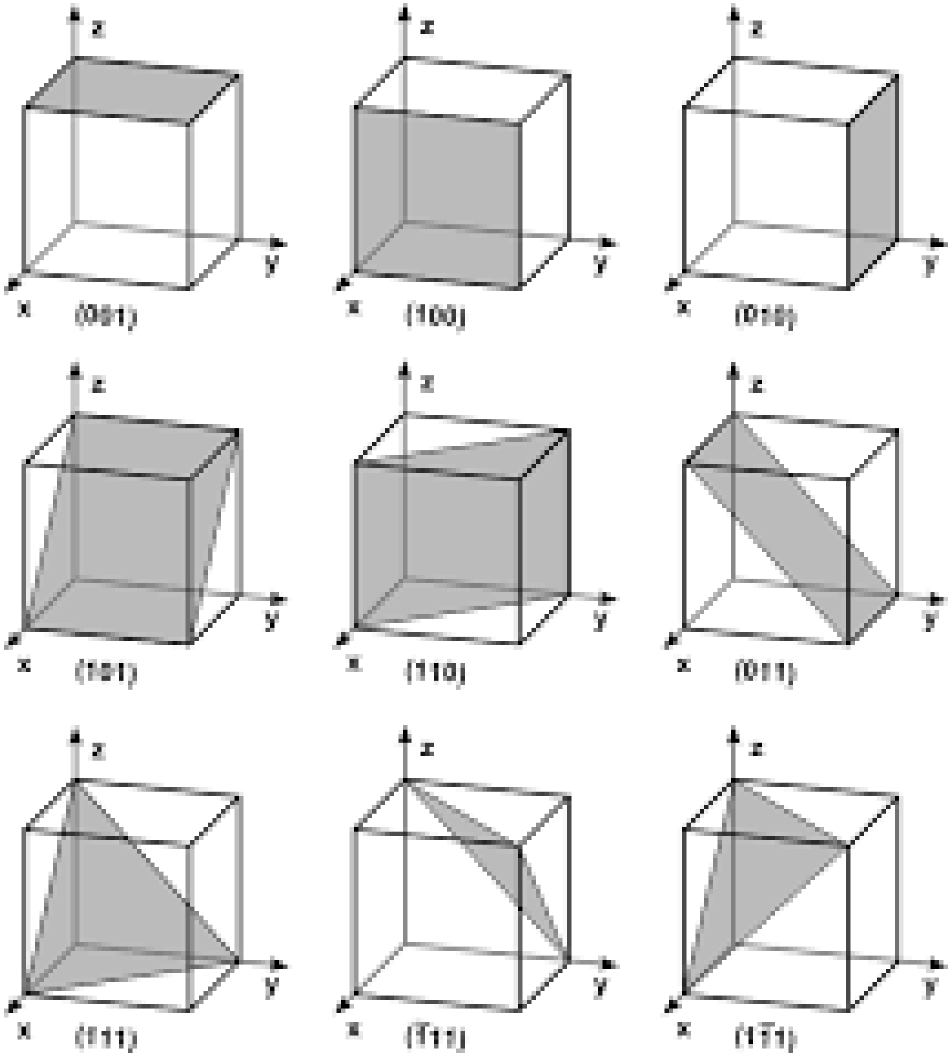


(100) (110) (111)

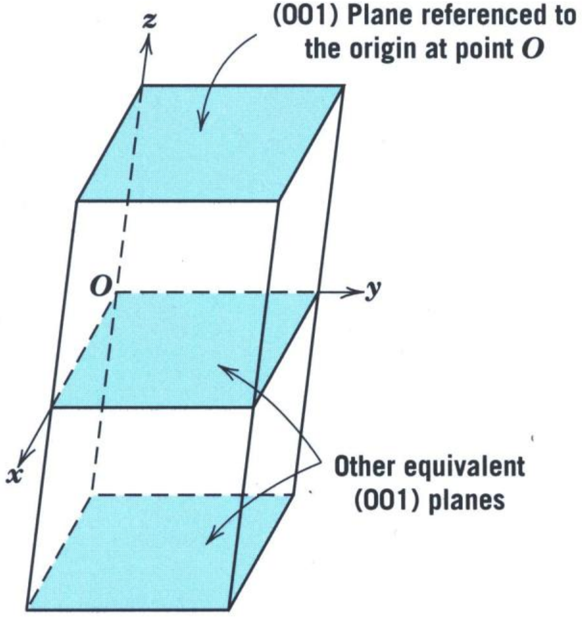
(200) ($\bar{1}00$)

Figure 16 Indices of important planes in a cubic crystal. The plane (200) is parallel to (100) and to ($\bar{1}00$).

examples



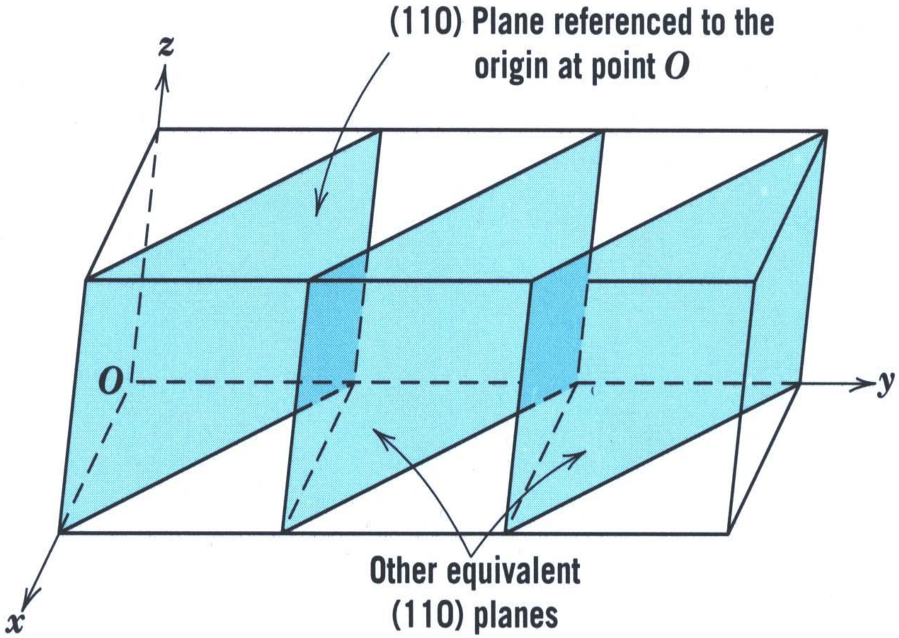
001 Plane



z
(001) Plane referenced to the origin at point O
O
y
x
Other equivalent (001) planes

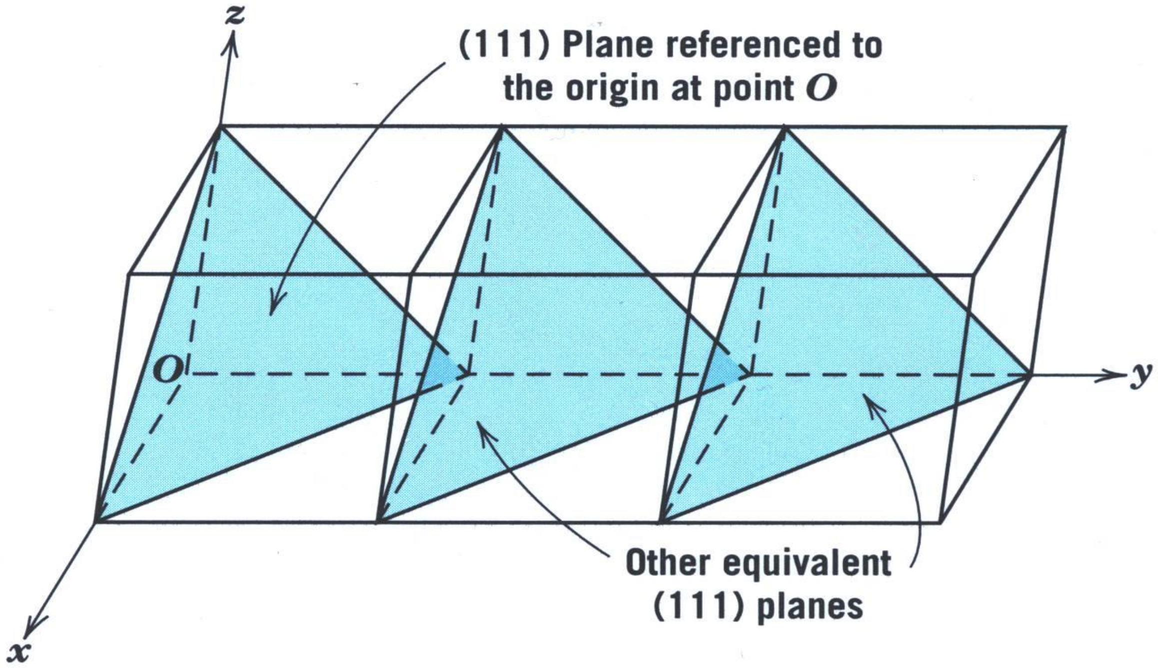
(a)

110 Planes


(110) Plane referenced to the origin at point *O*
z
O
y
x
Other equivalent (110) planes

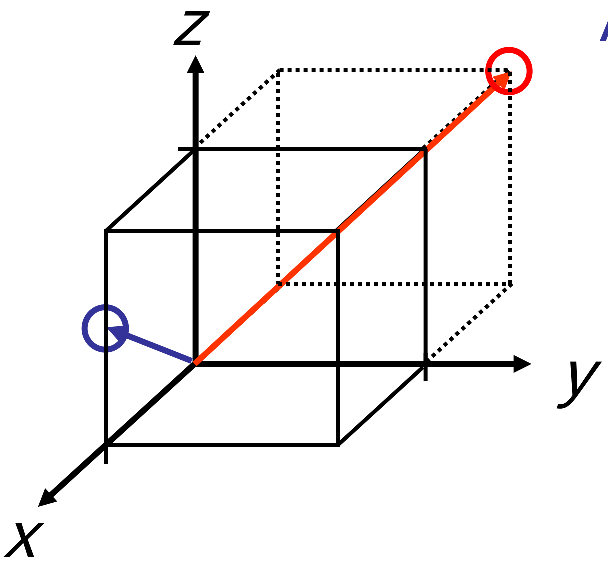
(b)

111 Planes


z
(111) Plane referenced to the origin at point O
O
y
x
Other equivalent (111) planes

(c)

Crystallographic Directions



Algorithm

1. Vector is repositioned (if necessary) to ***pass through the Unit Cell origin***.
2. Read off line projections (to principal axes of U.C.) in terms of unit cell dimensions *a*, *b*, and *c*
3. Adjust to smallest **integer values**
4. Enclose in square brackets, *no commas*

[*uvw*]

ex: 1, 0, ½ => 2, 0, 1 => [201]

-1, 1, 1 => $[\bar{1}11]$ where 'overbar' represents a negative index

families of directions <*uvw*>

d -spacing

$$d_{hkl} = \frac{n}{\sqrt{\frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}}}$$

$$d_{hkl} = \frac{a}{\sqrt{h\wedge 2 + k\wedge 2 + l\wedge 2}}$$

Example

The lattice constant for aluminum is 4.041 angstroms. What is d_{220}?

$$d_{hkl} = \frac{1}{\sqrt{\frac{h^2 + k^2}{a^2}}} = \frac{1}{\sqrt{\frac{2^2 + 2^2}{4.041^2}}} = 1.43 \text{ angstroms}$$

Theoretical Density, ρ

$$\text{Density} = \rho = \frac{\text{Mass of Atoms in Unit Cell}}{\text{Total Volume of Unit Cell}}$$

$$\rho = \frac{n\,A}{V_C N_A}$$

where n = number of atoms/unit cell

A = atomic weight

V_C = Volume of unit cell = a^3 for cubic

N_A = Avogadro's number

= 6.023×10^{23} atoms/mol

Number of atoms per unit cell

Coordination Number

- For a Bravais Lattice,

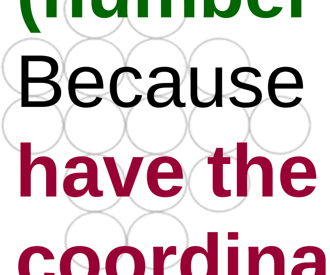
  Coordination Number ≡ **The number of lattice points closest to a given point**

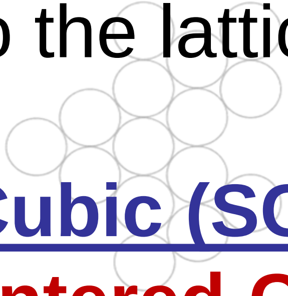
  (number of nearest-neighbors of each point).

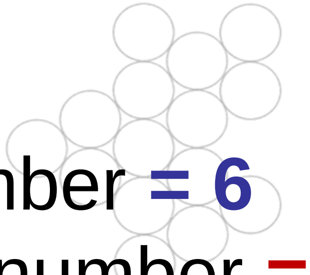
- Because of lattice periodicity, **all lattice points have the same** number of nearest neighbors or **coordination number**. (Coordination number is intrinsic to the lattice.)

Examples

1. **Simple Cubic (SC)** coordination number **= 6**
2. **Body-Centered Cubic** coordination number **= 8**
3. **Face-Centered Cubic** coordination number **= 12**







Arrangement of lattice points in the unit cell & No. of Lattice points / cell

		Position of lattice points	Effective number of Lattice points / cell
1	P	8 Corners	= 8 x (1/8) = 1
2	I	8 Corners + 1 body centre	= 1 (for corners) + 1 (BC)
3	F	8 Corners + 6 face centres	= 1 (for corners) + 6 x (1/2) = 4
4	A/ B/ C	8 corners + 2 centres of opposite faces	= 1 (for corners) + 2x(1/2) = 2

Atomic Packing Factor (Packing Fraction)

- For a Bravais Lattice,

The Atomic Packing Factor (APF) ≡

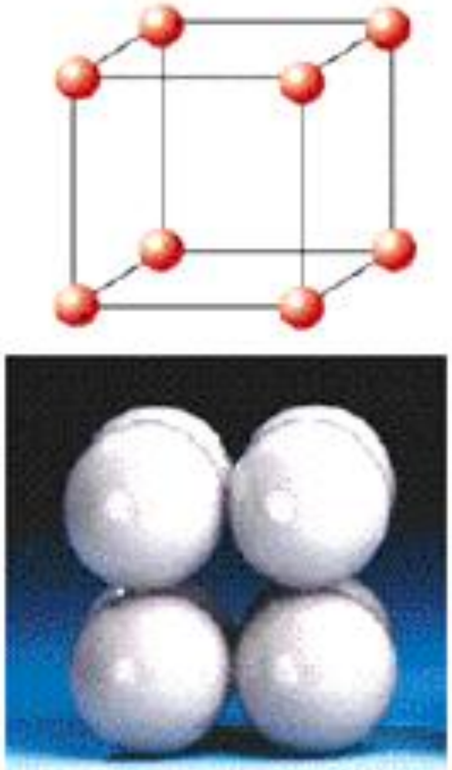
volume of the atoms within the unit cell divided by the volume of the unit cell.

$$\mathrm{APF} = \frac{\text{Volume of Atoms in Unit Cell}}{\text{Volume of Unit Cell}}$$

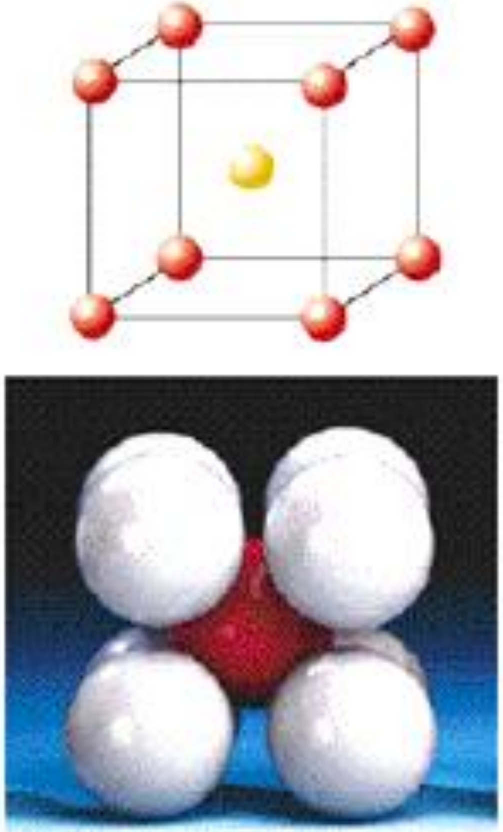
- When calculating the APF, the volume of the atoms in the unit cell is calculated *AS IF each atom was a hard sphere*, centered on the lattice point & large enough to just touch the nearest-neighbor sphere.
- Of course, from Quantum Mechanics, we know that this is very unrealistic for any atom!!

1- CUBIC CRYSTAL SYSTEMS

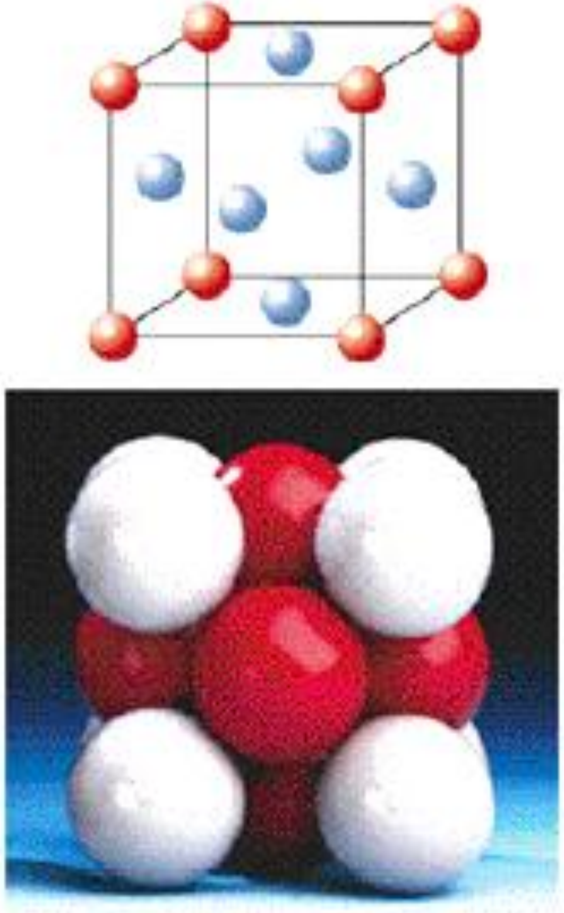
3 Common Unit Cells with *Cubic Symmetry*



Simple Cubic (SC)



Body Centered Cubic (BCC)



Face Centered Cubic (FCC)

3 Common Unit Cells with *Cubic Symmetry*

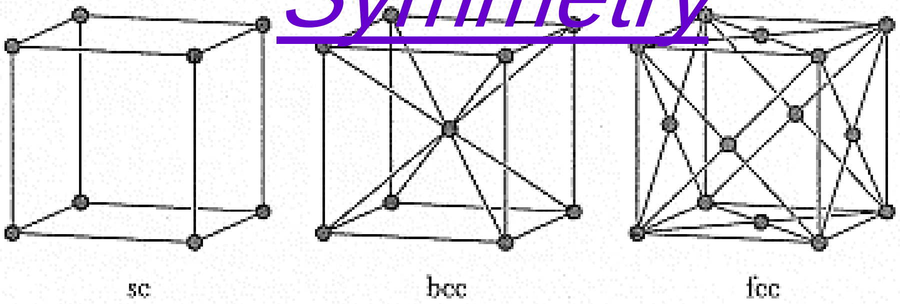


Figure 8 The cubic space lattices. The cells shown are the conventional cells.

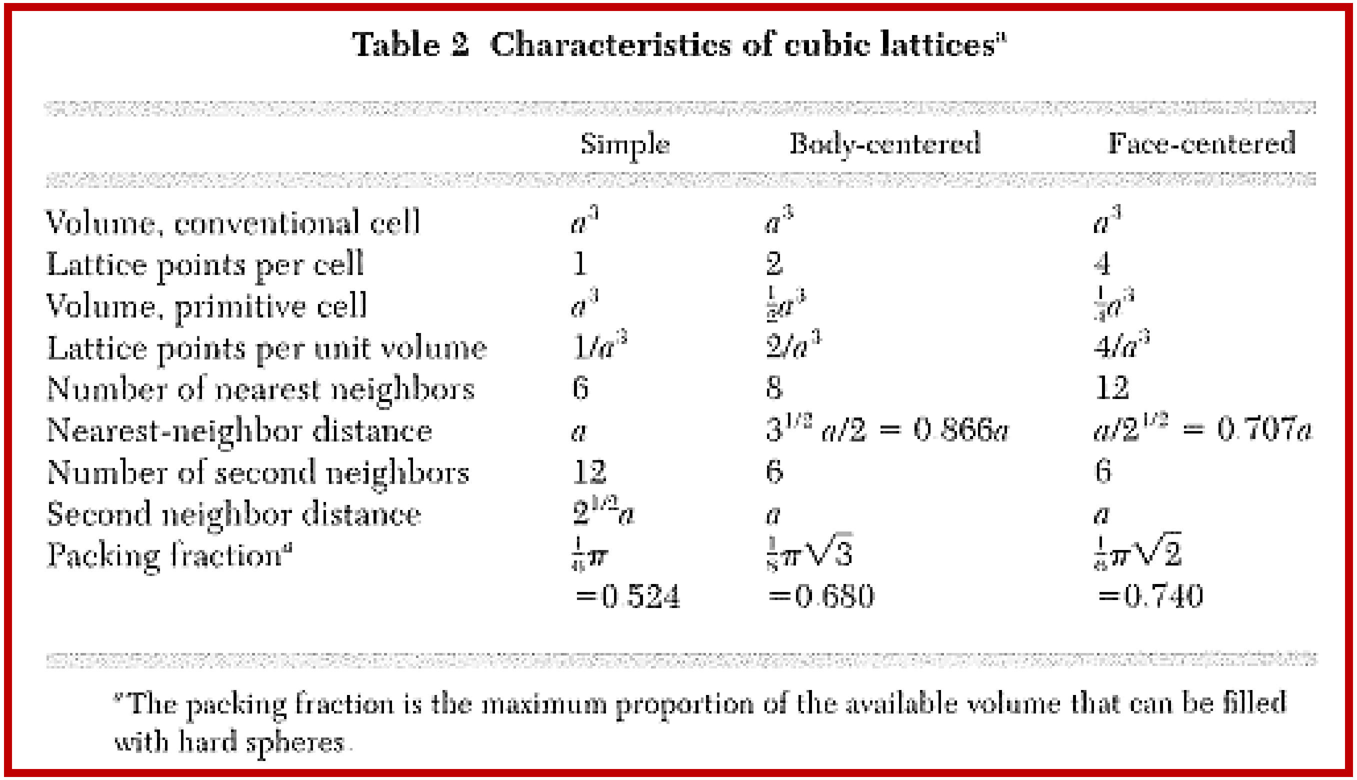


Table 2 Characteristics of cubic lattices[a]

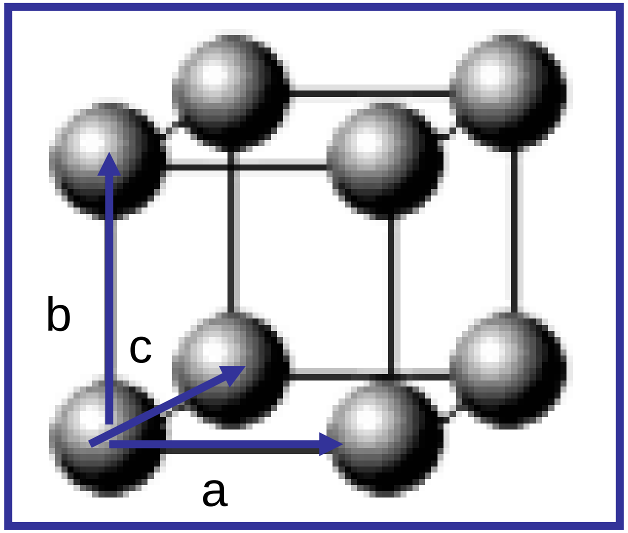
	Simple	Body-centered	Face-centered
Volume, conventional cell	a^3	a^3	a^3
Lattice points per cell	1	2	4
Volume, primitive cell	a^3	$\frac{1}{2}a^3$	$\frac{1}{4}a^3$
Lattice points per unit volume	$1/a^3$	$2/a^3$	$4/a^3$
Number of nearest neighbors	6	8	12
Nearest-neighbor distance	a	$3^{1/2}a/2 = 0.866a$	$a/2^{1/2} = 0.707a$
Number of second neighbors	12	6	6
Second neighbor distance	$2^{1/2}a$	a	a
Packing fraction[a]	$\frac{1}{6}\pi$ $=0.524$	$\frac{1}{8}\pi\sqrt{3}$ $=0.680$	$\frac{1}{6}\pi\sqrt{2}$ $=0.740$

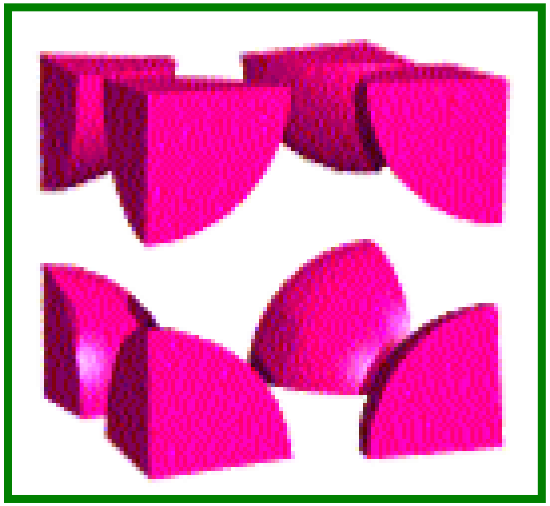
[a] The packing fraction is the maximum proportion of the available volume that can be filled with hard spheres.

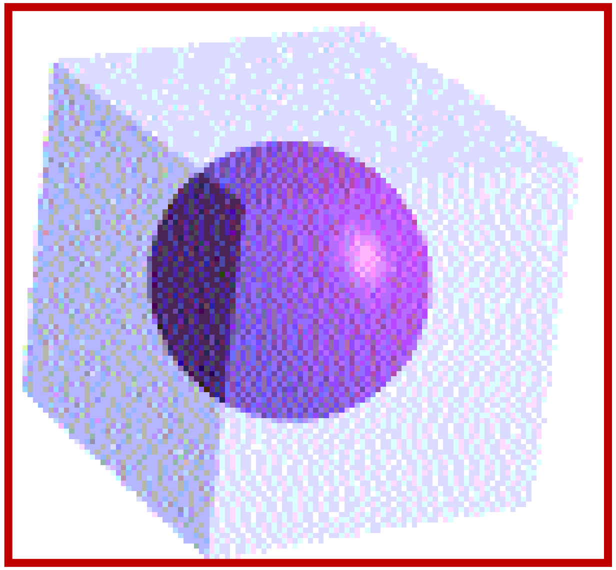
a- Simple Cubic (SC) Lattice

- The SC Lattice has one lattice point in its unit cell, so it’s unit cell is a primitive cell.
- In the unit cell on the left, the atoms at the corners are cut because only a portion (in this case 1/8) “belongs” to that cell. The rest of the atom “belongs” to neighboring cells.

Coordinatination Number of the SC Lattice = 6.

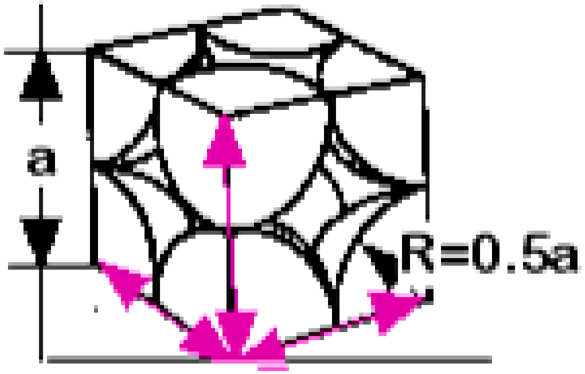






Simple Cubic (SC) Lattice

Atomic Packing Factor



close-packed directions

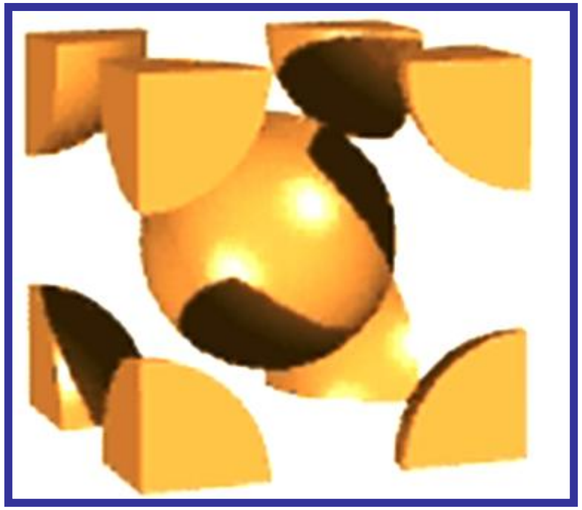
contains 8 x 1/8 =
1atom/unit cell

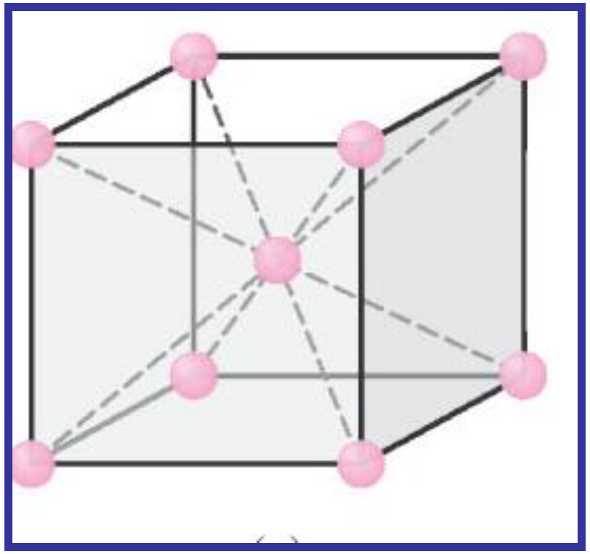
APF = 0.52 for simple cubic

$$\mathrm{APF} = \frac{\underset{\frac{\text{atom}}{\text{unit cell}}}{\boxed{1}}\;\underset{\frac{\text{volume}}{\text{atom}}}{\boxed{\frac{4}{3}\pi(0.5a)^3}}}{\underset{\frac{\text{volume}}{\text{unit cell}}}{\boxed{a^3}}}$$

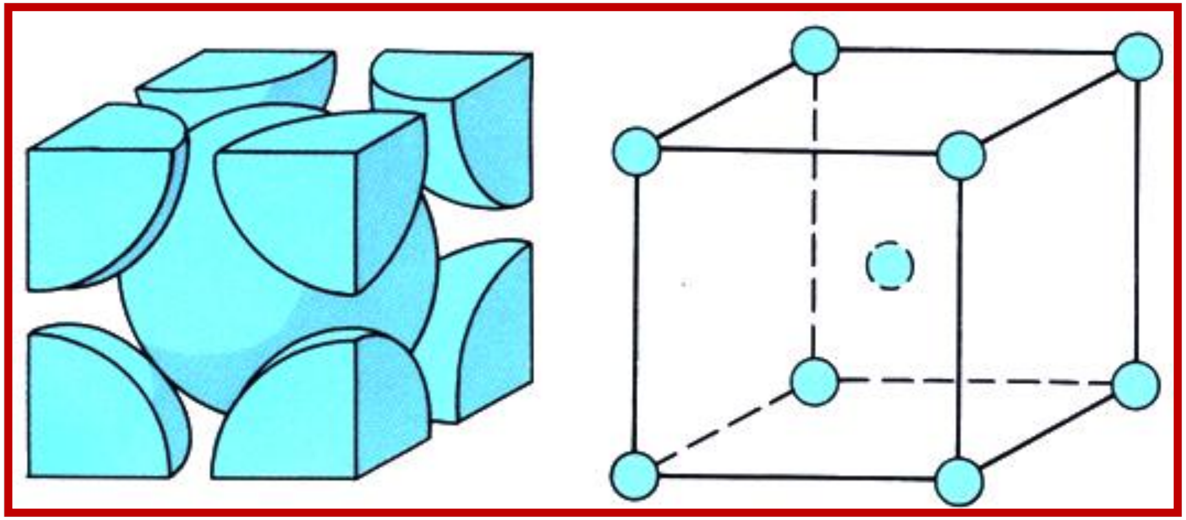
b- Body Centered Cubic (BCC) Lattice

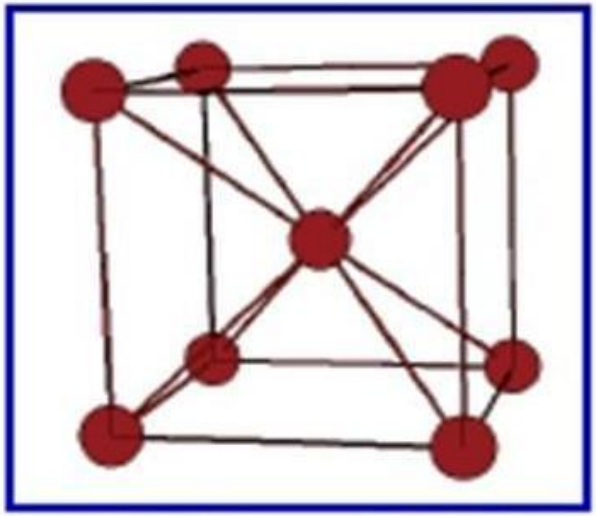
- The BCC Lattice has two lattice points per unit cell so the BCC unit cell is a non-primitive cell.
- Every BCC lattice point has 8 nearest- neighbors. So (in the hard sphere model) each atom is in contact with its neighbors only along the body-diagonal directions.
- Many metals (Fe,Li,Na..etc), including the alkalis and several transition elements have the BCC structure.



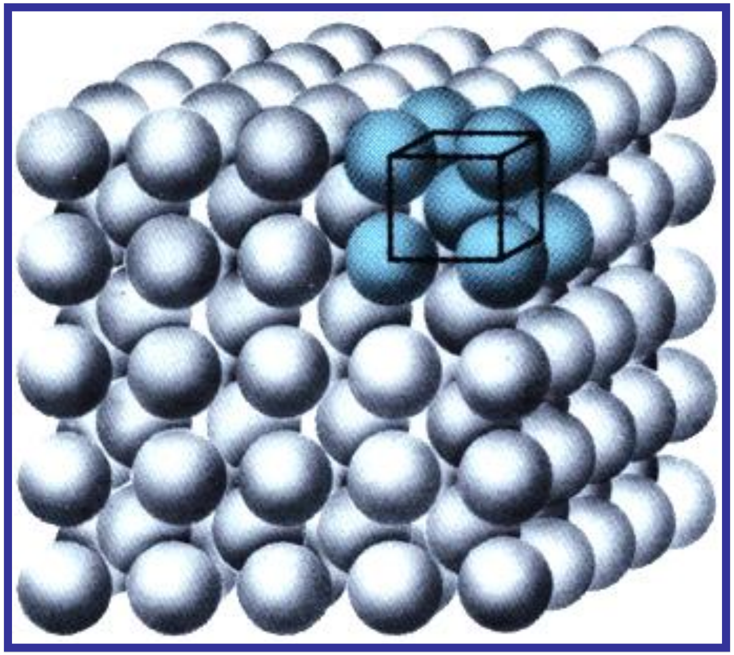


Body Centered Cubic (BCC) Structure





Body Centered Cubic and related structures



Body Centered Cubic (BCC) Lattice

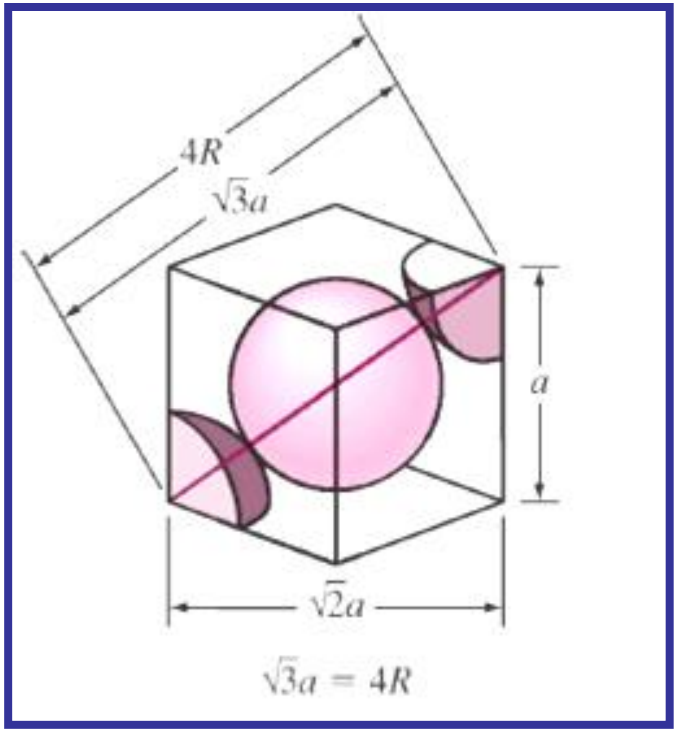
Atomic Packing Factor

$\frac{\text{atom}}{\text{unit cell}}$

$\frac{\text{volume}}{\text{atom}}$

$$APF = \frac{2 \; \frac{4}{3}\pi(0.433a)}{a^3}$$

$\frac{\text{volume}}{\text{unit cell}}$



$$APF_{BCC} = \frac{V_{atoms}}{V_{unitcell}} = 0.68$$

Elements That Form Solids with the BCC Structure

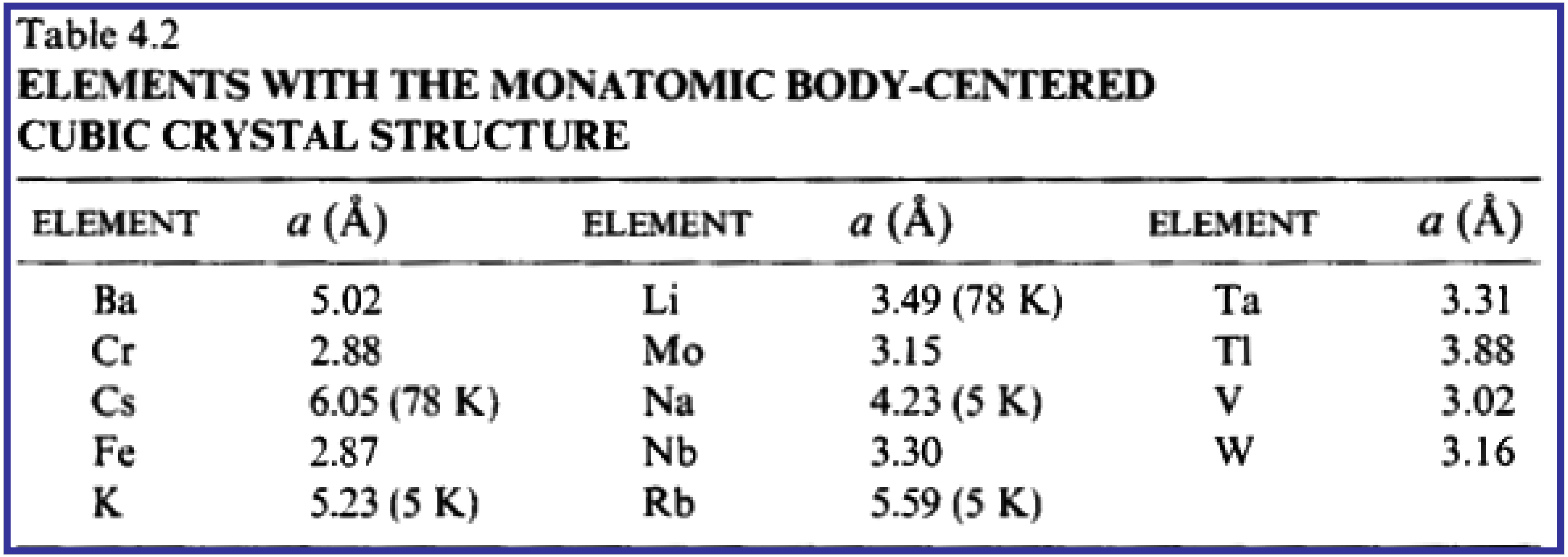


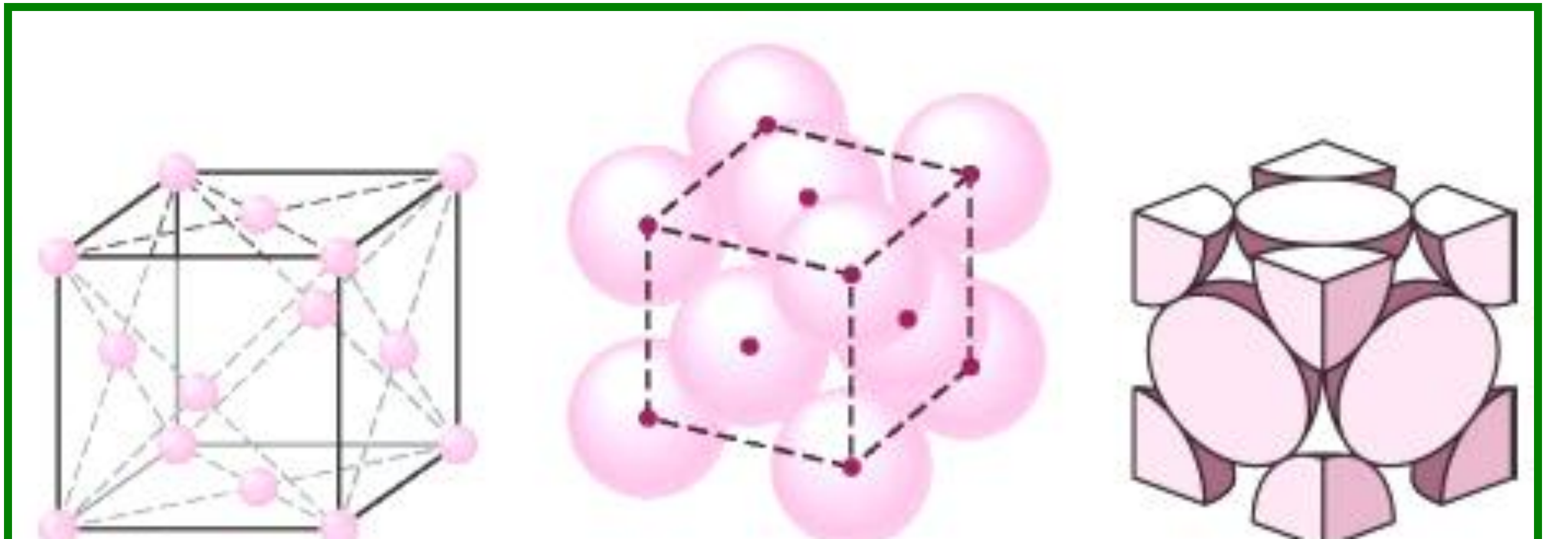
Table 4.2

ELEMENTS WITH THE MONATOMIC BODY-CENTERED CUBIC CRYSTAL STRUCTURE

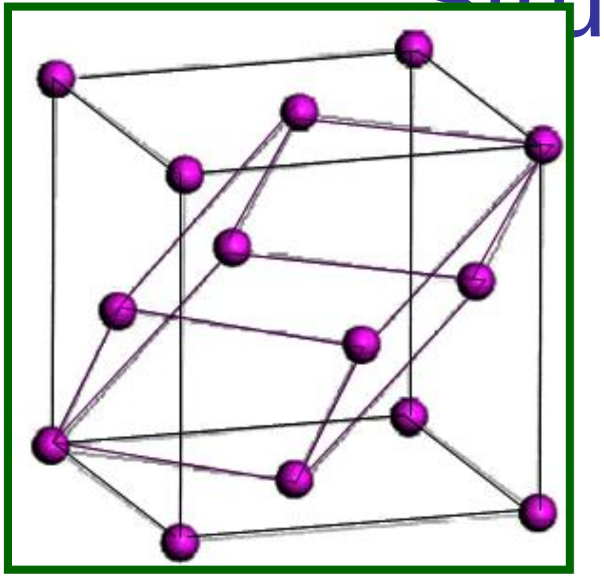
ELEMENT	*a* (Å)	ELEMENT	*a* (Å)	ELEMENT	*a* (Å)
Ba	5.02	Li	3.49 (78 K)	Ta	3.31
Cr	2.88	Mo	3.15	Tl	3.88
Cs	6.05 (78 K)	Na	4.23 (5 K)	V	3.02
Fe	2.87	Nb	3.30	W	3.16
K	5.23 (5 K)	Rb	5.59 (5 K)		

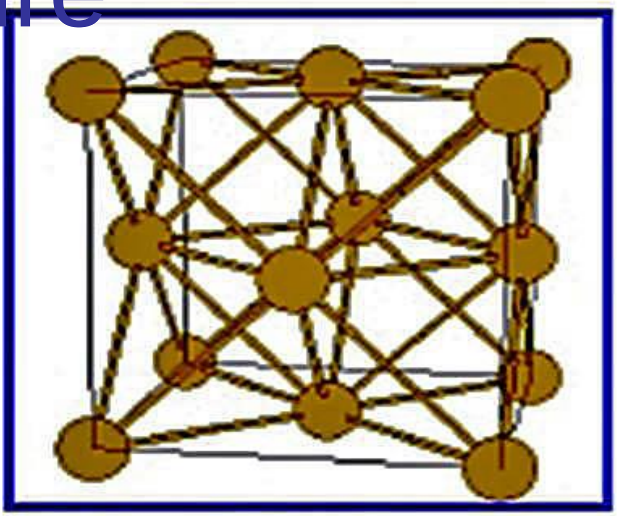
c- Face Centered Cubic (FCC) Lattice

- In the **FCC Lattice** there are atoms at the corners of the unit cell and at the center of each face.
- The FCC unit cell has 4 atoms so it is a non-primitive cell.
- Every **FCC Lattice** point has 12 nearest-neighbors.
- **Many common metals** (**Cu,Ni,Pb..**etc) crystallize in the **FCC structure.**

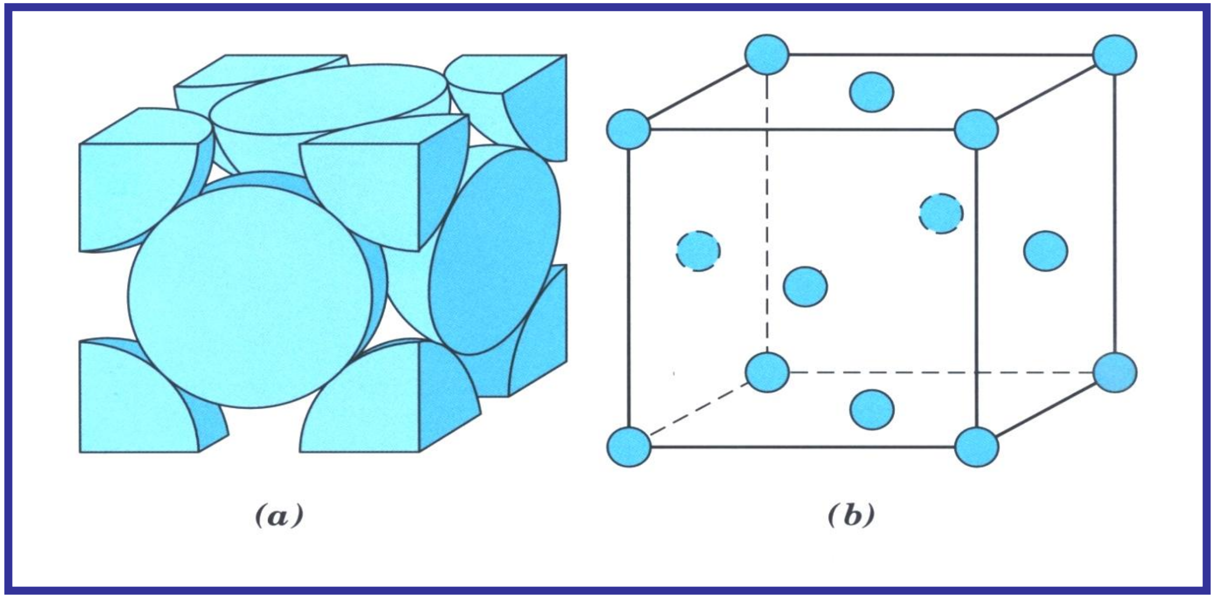


Face Centered Cubic (FCC) Structure





A1 (fcc) Structure



(a) (b)

Closed-packed structures

(or, what does stacking fruit have to do with solid state physics?)

FCC: Conventional Cell With Basis

- We can also view the FCC lattice in terms of a conventional unit cell with a four point basis.

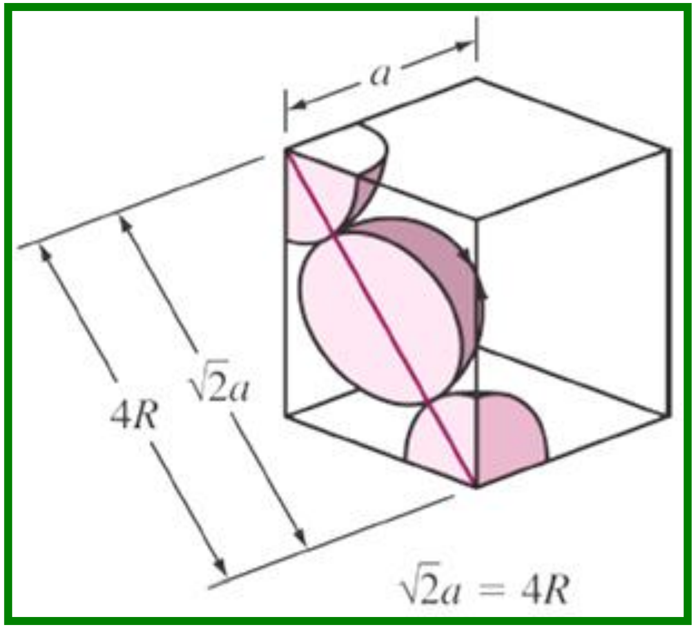
- Similarly, we can view the BCC lattice in terms of a conventional unit cell with a two point basis.

Simple Crystal Structures

- There are several crystal structures of common interest: sodium chloride, cesium chloride, hexagonal close-packed, diamond and cubic zinc sulfide.
- Each of these structures have many different realizations.

Face Centered Cubic (FCC) Lattice

Atomic Packing Factor



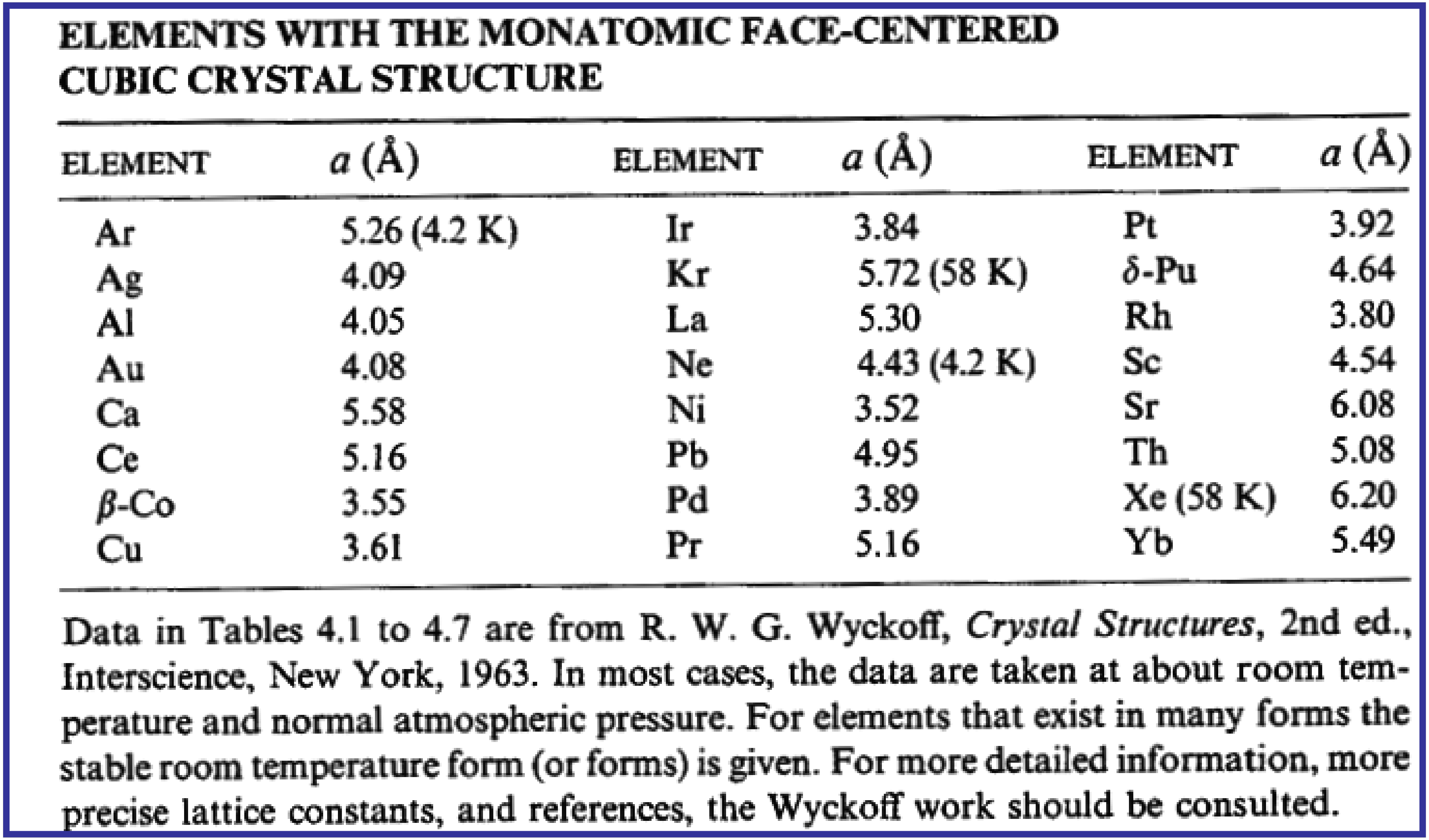
$$\frac{\text{atom}}{\text{unit cell}} \qquad \frac{\text{volume}}{\text{atom}}$$

$$\text{APF} = \frac{4\left(\frac{4}{3}\pi(0.353a)\right)}{a^3}$$

$$\frac{\text{volume}}{\text{unit cell}}$$

$$APF_{FCC} = \frac{V_{atoms}}{V_{unitcell}} = 0.74$$

Elements That Form Solids with the FCC Structure



ELEMENTS WITH THE MONATOMIC FACE-CENTERED CUBIC CRYSTAL STRUCTURE

ELEMENT	a (Å)	ELEMENT	a (Å)	ELEMENT	a (Å)
Ar	5.26 (4.2 K)	Ir	3.84	Pt	3.92
Ag	4.09	Kr	5.72 (58 K)	δ-Pu	4.64
Al	4.05	La	5.30	Rh	3.80
Au	4.08	Ne	4.43 (4.2 K)	Sc	4.54
Ca	5.58	Ni	3.52	Sr	6.08
Ce	5.16	Pb	4.95	Th	5.08
β-Co	3.55	Pd	3.89	Xe (58 K)	6.20
Cu	3.61	Pr	5.16	Yb	5.49

Data in Tables 4.1 to 4.7 are from R. W. G. Wyckoff, *Crystal Structures*, 2nd ed., Interscience, New York, 1963. In most cases, the data are taken at about room temperature and normal atmospheric pressure. For elements that exist in many forms the stable room temperature form (or forms) is given. For more detailed information, more precise lattice constants, and references, the Wyckoff work should be consulted.

FCC & BCC:
Conventional Cells With a Basis

- Alternatively, **the FCC Lattice** can be viewed in terms of a ***Conventional Unit Cell with a 4-point basis*****.**
- Similarly, **the BCC lattice** can be viewed in terms of a ***Conventional Unit Cell with a 2-point basis.***

Comparison of the 3 Cubic Lattice Systems

Unit Cell Contents

Counting the number of atoms *within* the unit cell

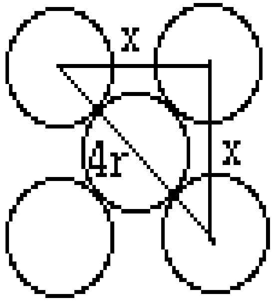
Atom Position	Shared Between	Each atom counts:
corner	8 cells	1/8
face center	2 cells	1/2
body center	1 cell	1
edge center	2 cells	1/2

Lattice Type	Atoms per Cell
P (Primitive)	1 [= 8 × 1/8]
I (Body Centered)	2 [= (8 × 1/8) + (1 × 1)]
F (Face Centered)	4 [= (8 × 1/8) + (6 × 1/2)]
C (Side Centered)	2

Example: Atomic Packing Factor

It is very easy to show that the filling of space by spheres is 74%
e.g. for the fcc unit cell of cubic close packing (CCP) with an ABC layer repeat

For spheres of radius, r, touching along the **face diagonal**, the cubic unit cell parameter is calculated as $x = 2\sqrt{2}\,r$



total unit cell volume $= x^3$

$= 16\sqrt{2}\,r^3$

occupied volume = 4 spheres

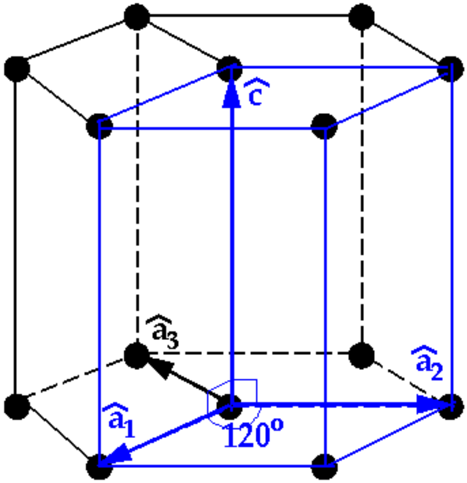
$= \frac{16\pi r^3}{3}$

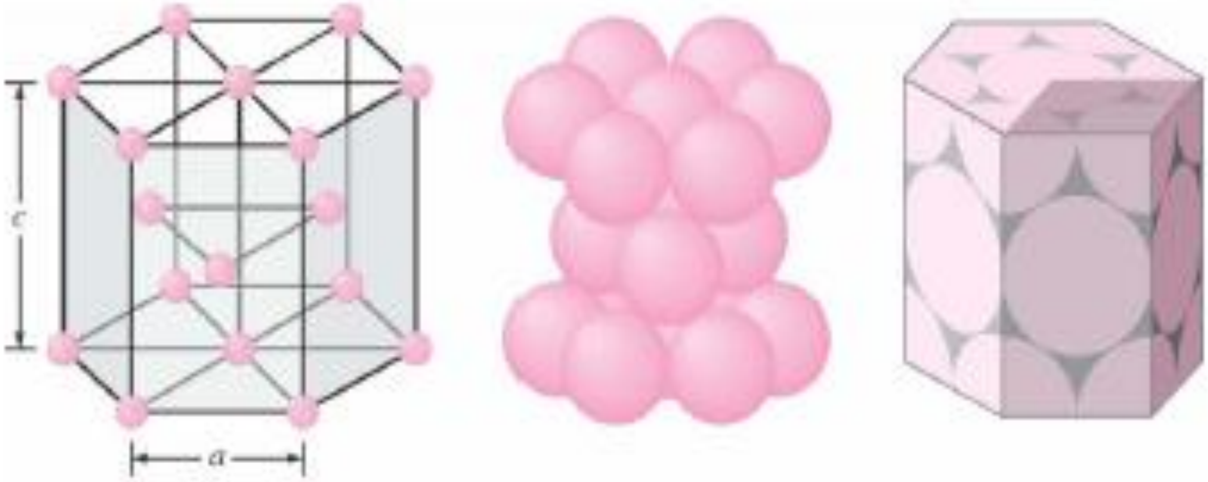
space filling $= \frac{\pi}{3\sqrt{2}}$ = **74.05 %**

2- HEXAGONAL CRYSTAL SYSTEMS

- In a *Hexagonal Crystal System*, three equal coplanar axes intersect at an angle of 60°, and another axis is perpendicular to the others and of a

r





The atoms are all the same.

Simple Hexagonal Bravais Lattice

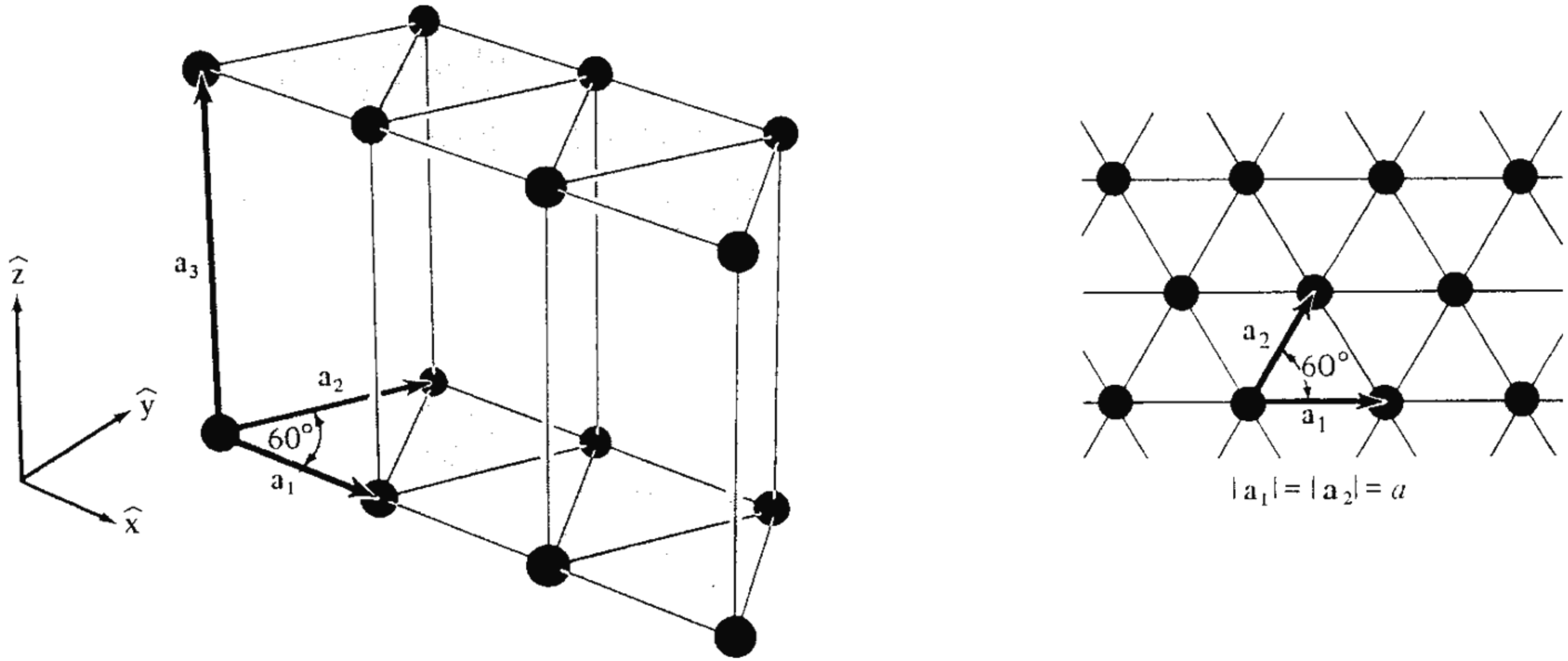
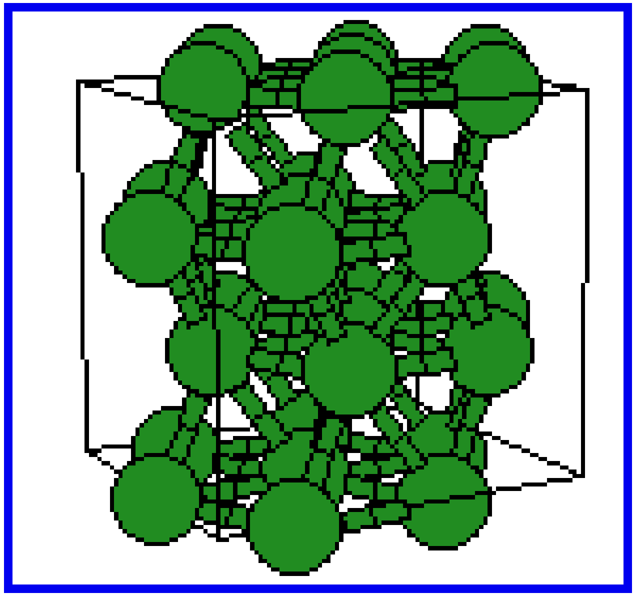
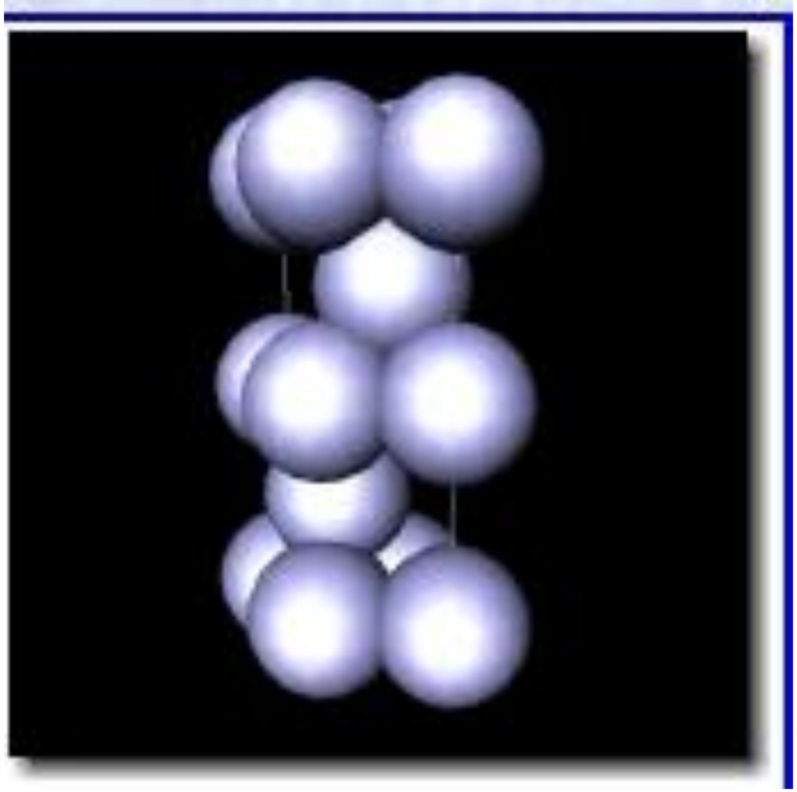


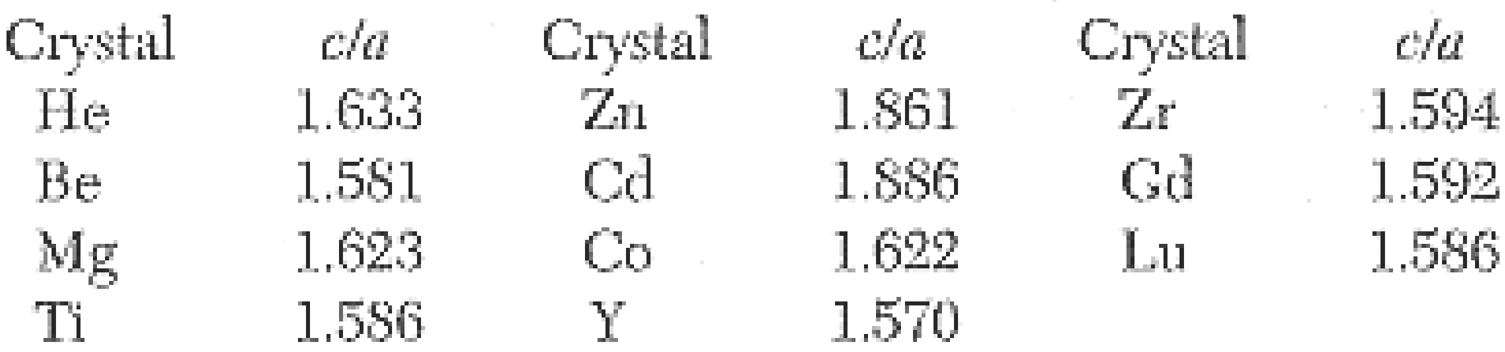
Figure 4.19
The simple hexagonal Bravais lattice. Two-dimensional triangular nets (shown in inset) are stacked directly above one another, a distance c apart.

Hexagonal Close Packed (HCP) Lattice



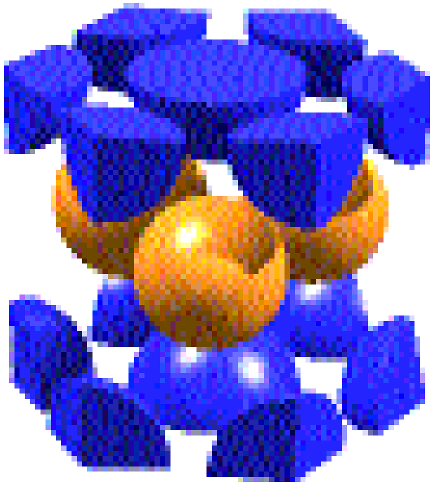
Hexagonal Close Packed and related structures

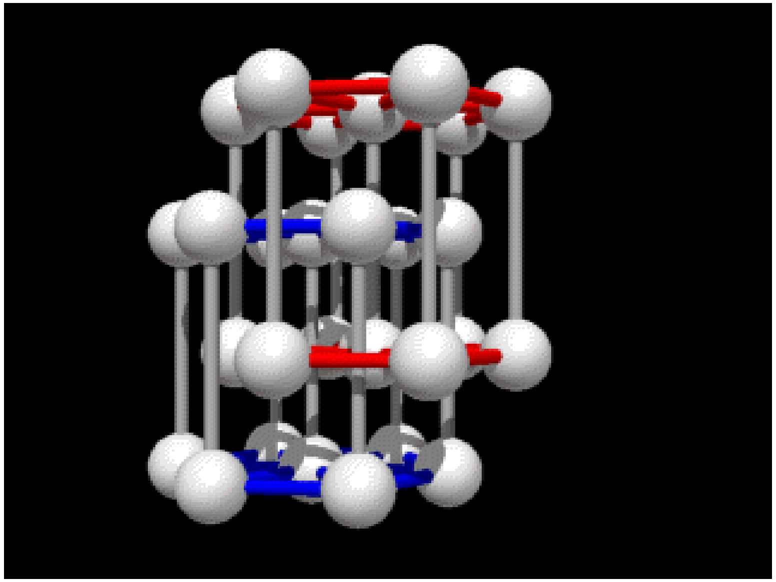




Crystal	*c/a*	Crystal	*c/a*	Crystal	*c/a*
He	1.633	Zn	1.861	Zr	1.594
Be	1.581	Cd	1.886	Gd	1.592
Mg	1.623	Co	1.622	Lu	1.586
Ti	1.586	Y	1.570		

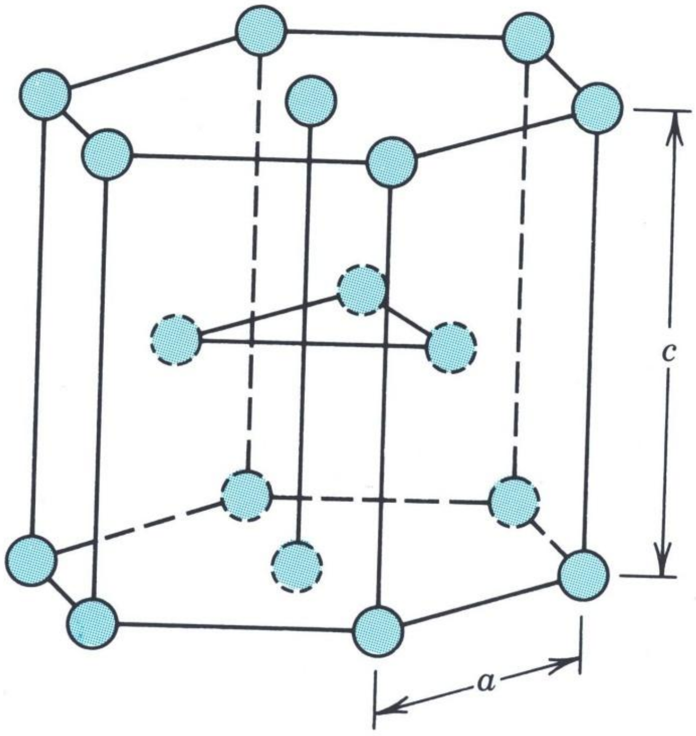
Hexagonal Close Packed (HCP) Lattice



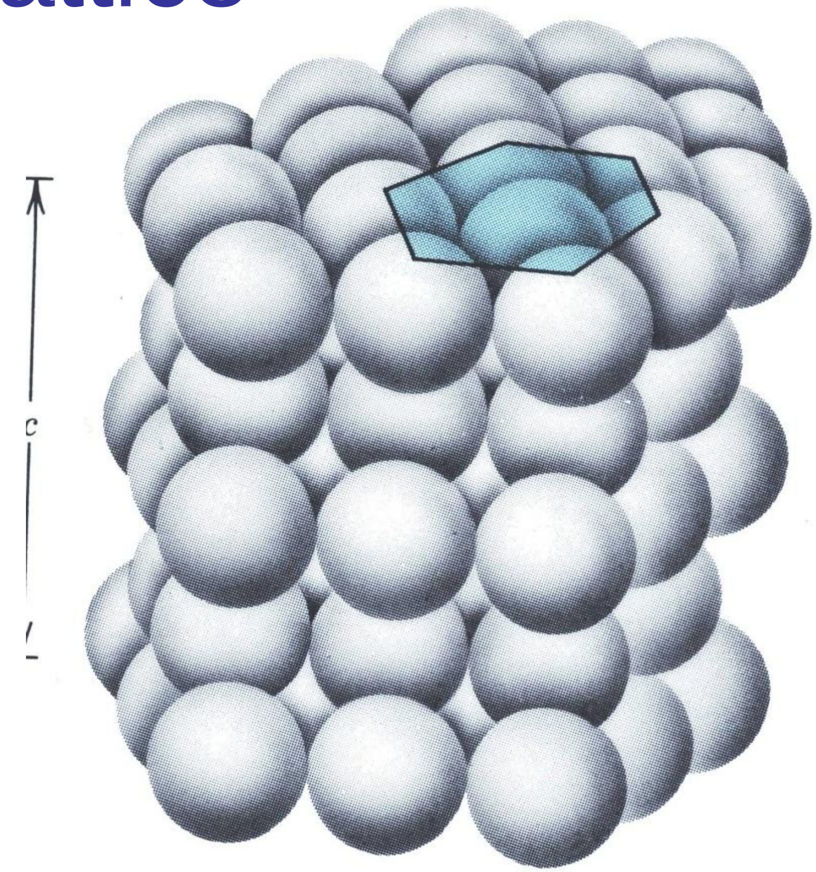


- This is another structure that is common, particularly in metals. In addition to the two layers of atoms which form the base and the upper face of the hexagon, there is also an intervening layer of atoms arranged such that each of these atoms rest over a depression between three atoms in

Hexagonal Close Packed (HCP) Lattice



(a)



(b)

The HCP lattice is not a Bravais lattice, because orientation of the environment of a point varies from layer to layer along the c-axis.

Hexagonal Close Packed (HCP) Lattice

Bravais Lattice:
Hexagonal Lattice

He, Be, Mg, Hf, Re

(Group II elements)

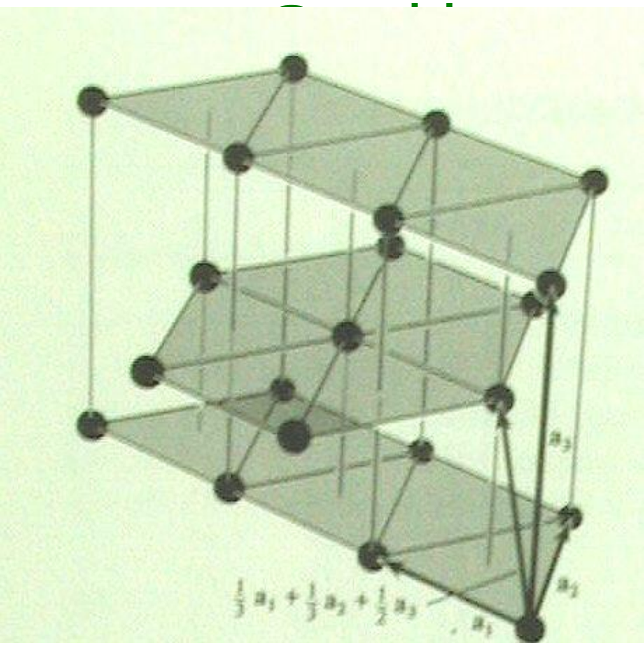
ABABAB Type of

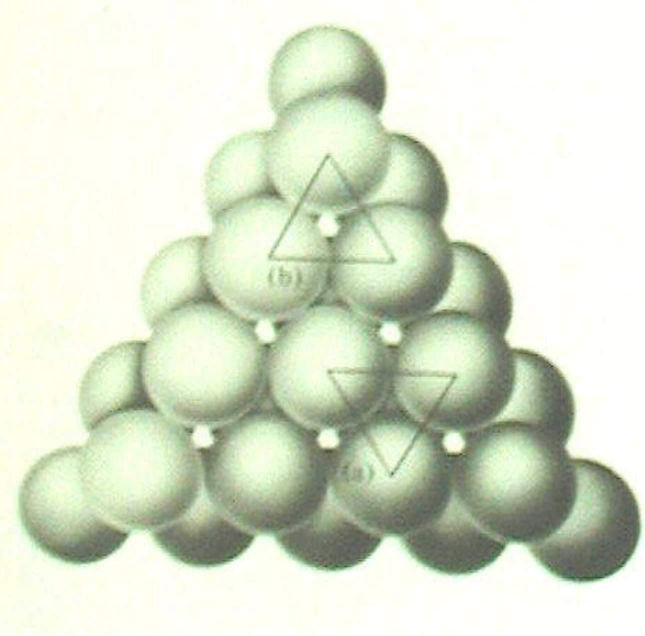
a = b

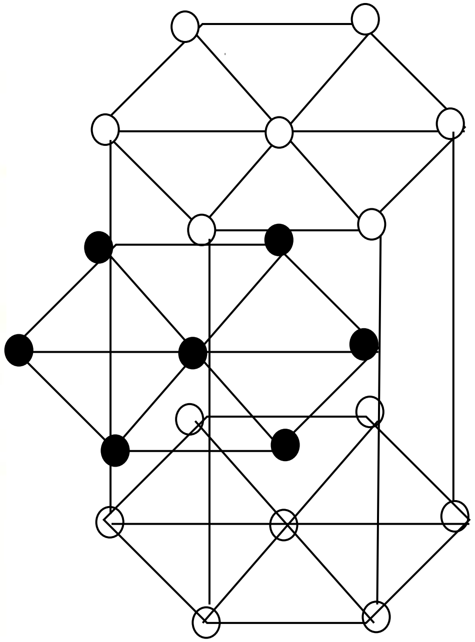
Angle between a & b = 120°

c = 1.633a,

Basis: (0,0,0) (2/3a ,1/3a,1/2c)

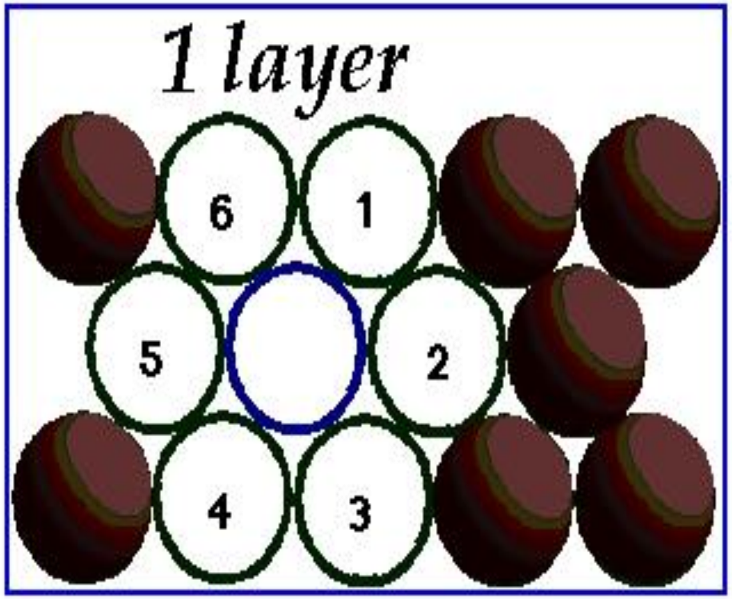






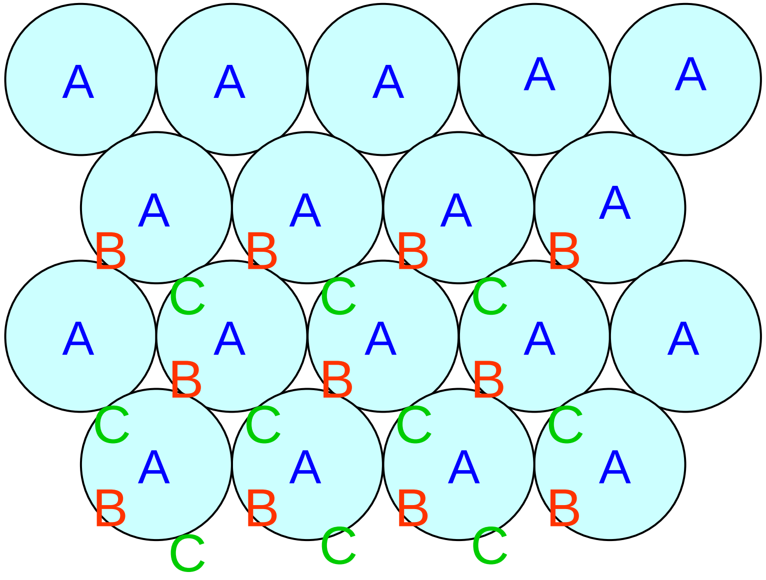
CLOSE-PACKING OF SPHERES

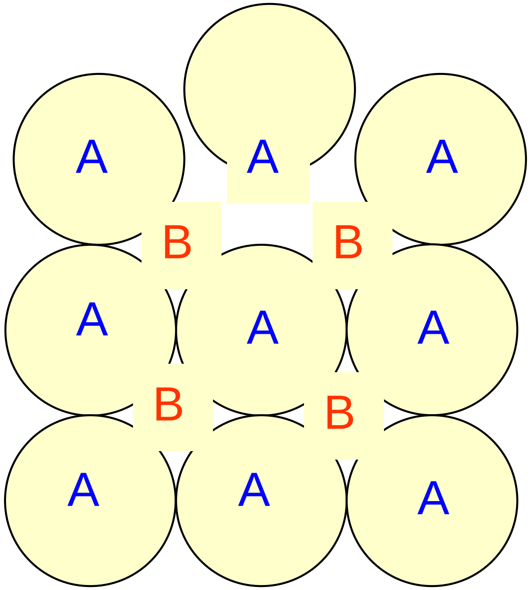
A *single layer* of spheres is closest-packed with a **HEXAGONAL** coordination of each sphere



Comments on Close Packing

Close Packed





Sequence ABCABCAB:
Face Centered Cubic
Close Packed

Sequence ABABAB:
Hexagonal Close
Packed

Sequence ABAB:
Body Centered Cubic

Sequence AAA:
Simple Cubic

Hexagonal Close Packing

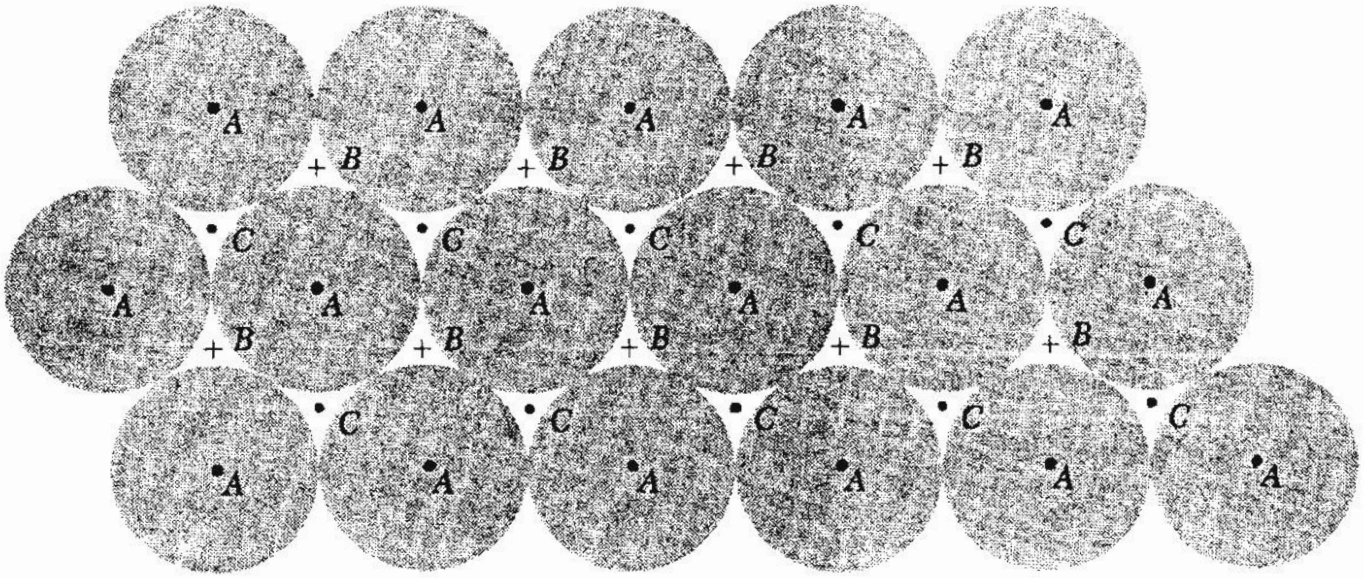


Figure 21 A close-packed layer of spheres is shown, with centers at points marked *A*. A second and identical layer of spheres can be placed on top of this, above and parallel to the plane of the drawing, with centers over the points marked *B*. There are two choices for a third layer. It can go in over *A* or over *C*. If it goes in over *A* the sequence is *ABABAB*. . . and the structure is hexagonal close-packed. If the third layer goes in over *C* the sequence is *ABCABCABC*. . . and the structure is face-centered cubic.

HCP Lattice ≡

Hexagonal Bravais Lattice with a 2 Atom Basis

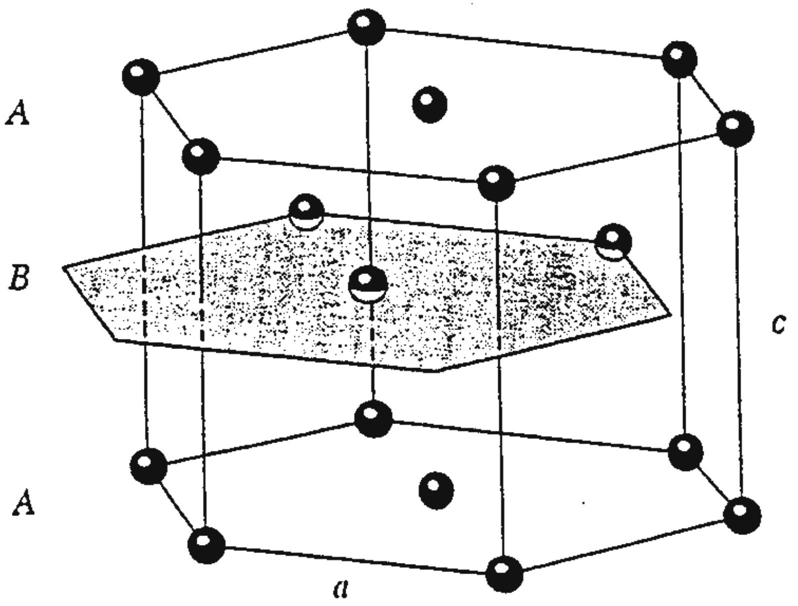
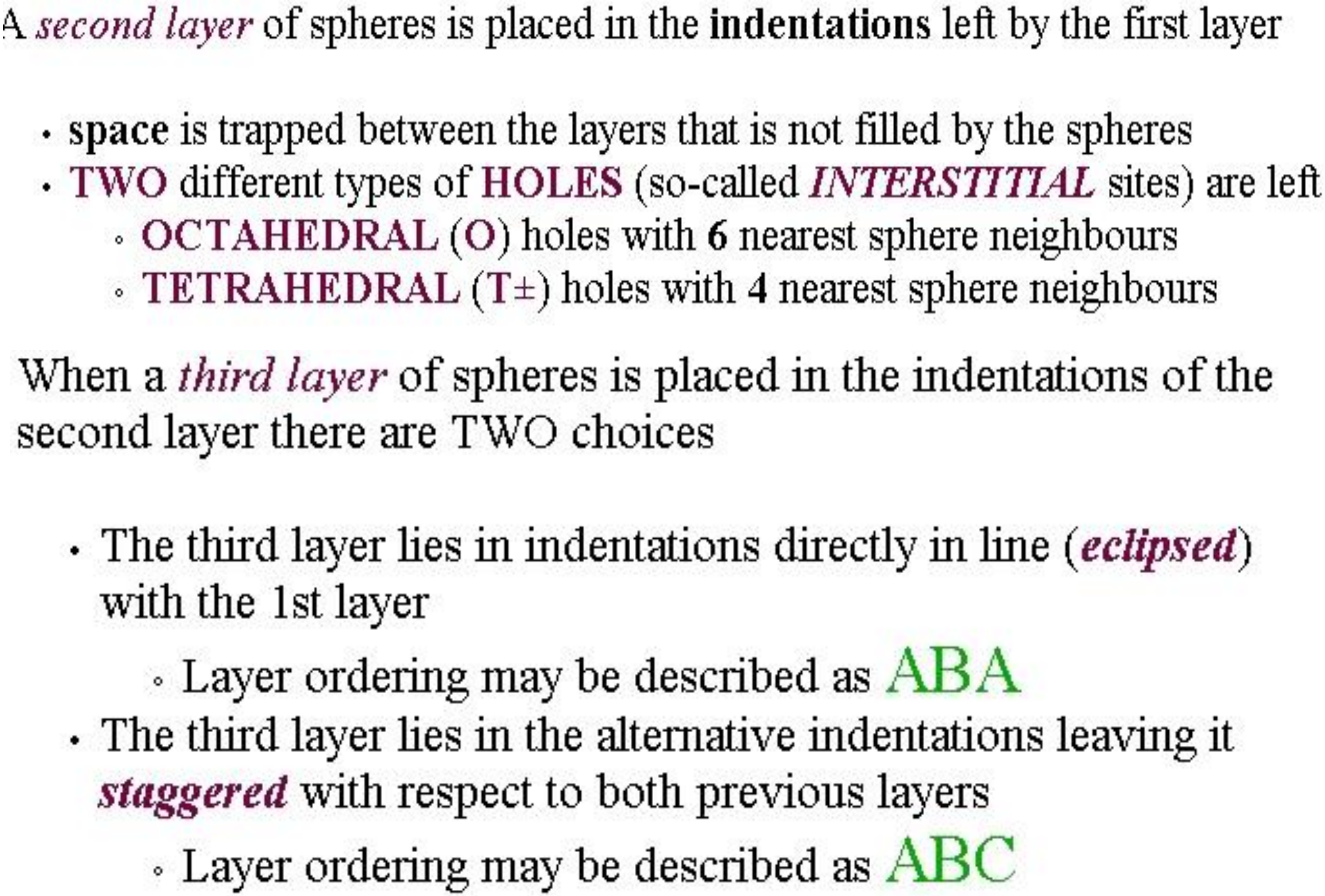


Figure 22 The hexagonal close-packed structure. The atom positions in this structure do not constitute a space lattice. The space lattice is simple hexagonal with a basis of two identical atoms associated with each lattice point. The lattice parameters *a* and *c* are indicated, where *a* is in the basal plane and *c* is the magnitude of the axis $\mathbf{a}_3$ of Fig. 14.

Comments on Close Packing

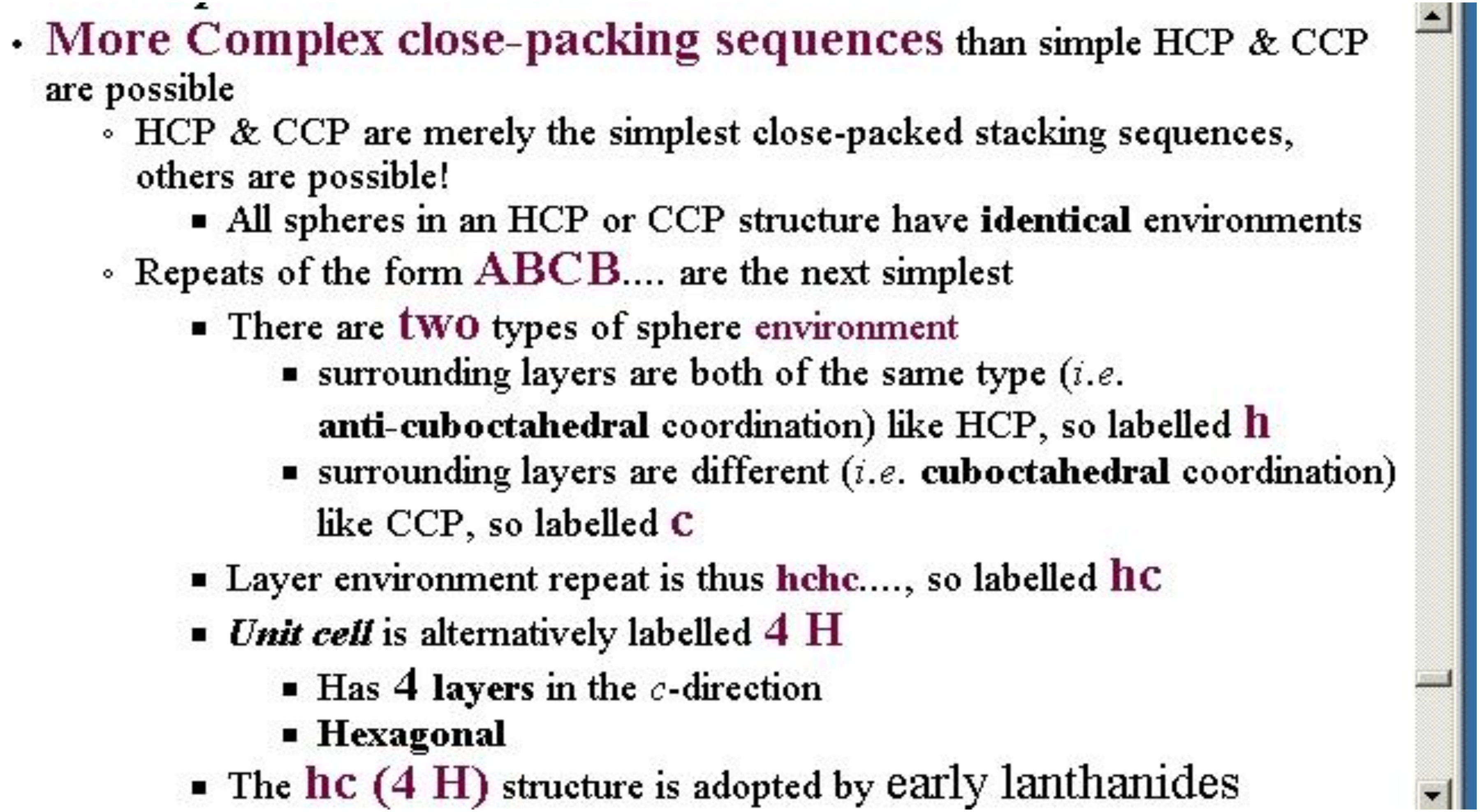


A *second layer* of spheres is placed in the **indentations** left by the first layer

- **space** is trapped between the layers that is not filled by the spheres
- **TWO** different types of **HOLES** (so-called ***INTERSTITIAL*** sites) are left
  - **OCTAHEDRAL** (**O**) holes with **6** nearest sphere neighbours
  - **TETRAHEDRAL** (**T±**) holes with **4** nearest sphere neighbours

When a *third layer* of spheres is placed in the indentations of the second layer there are TWO choices

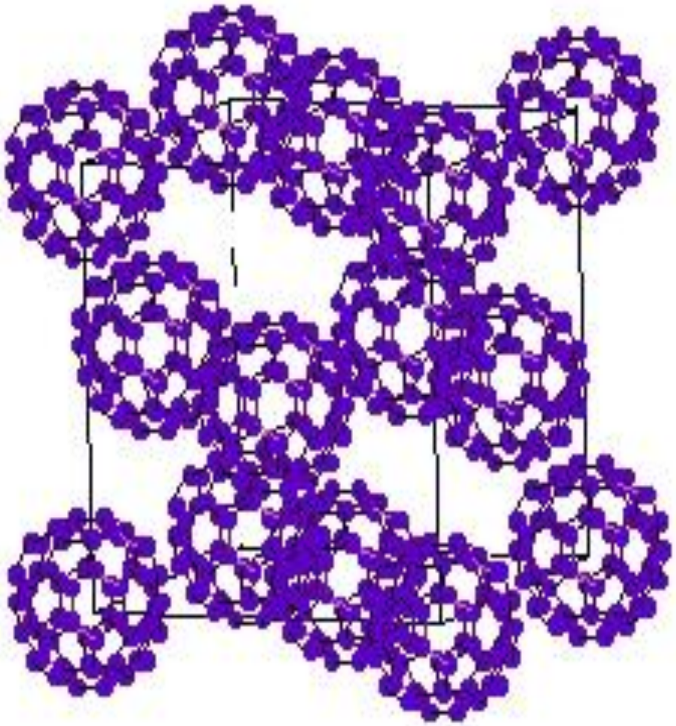
- The third layer lies in indentations directly in line (***eclipsed***) with the 1st layer
  - Layer ordering may be described as ABA
- The third layer lies in the alternative indentations leaving it ***staggered*** with respect to both previous layers
  - Layer ordering may be described as ABC



- More Complex close-packing sequences than simple HCP & CCP are possible
  - HCP & CCP are merely the simplest close-packed stacking sequences, others are possible!
    - All spheres in an HCP or CCP structure have **identical** environments
  - Repeats of the form ABCB.... are the next simplest
    - There are two types of sphere environment
      - surrounding layers are both of the same type (*i.e.* **anti-cuboctahedral** coordination) like HCP, so labelled h
      - surrounding layers are different (*i.e.* **cuboctahedral** coordination) like CCP, so labelled c
    - Layer environment repeat is thus **hchc**...., so labelled hc
    - ***Unit cell*** is alternatively labelled 4 H
      - Has 4 **layers** in the *c*-direction
      - **Hexagonal**
    - The hc (4 H) structure is adopted by early lanthanides

- Other Systems may be Classified as having Similar Structures

BUCKMINSTERFULLERENE

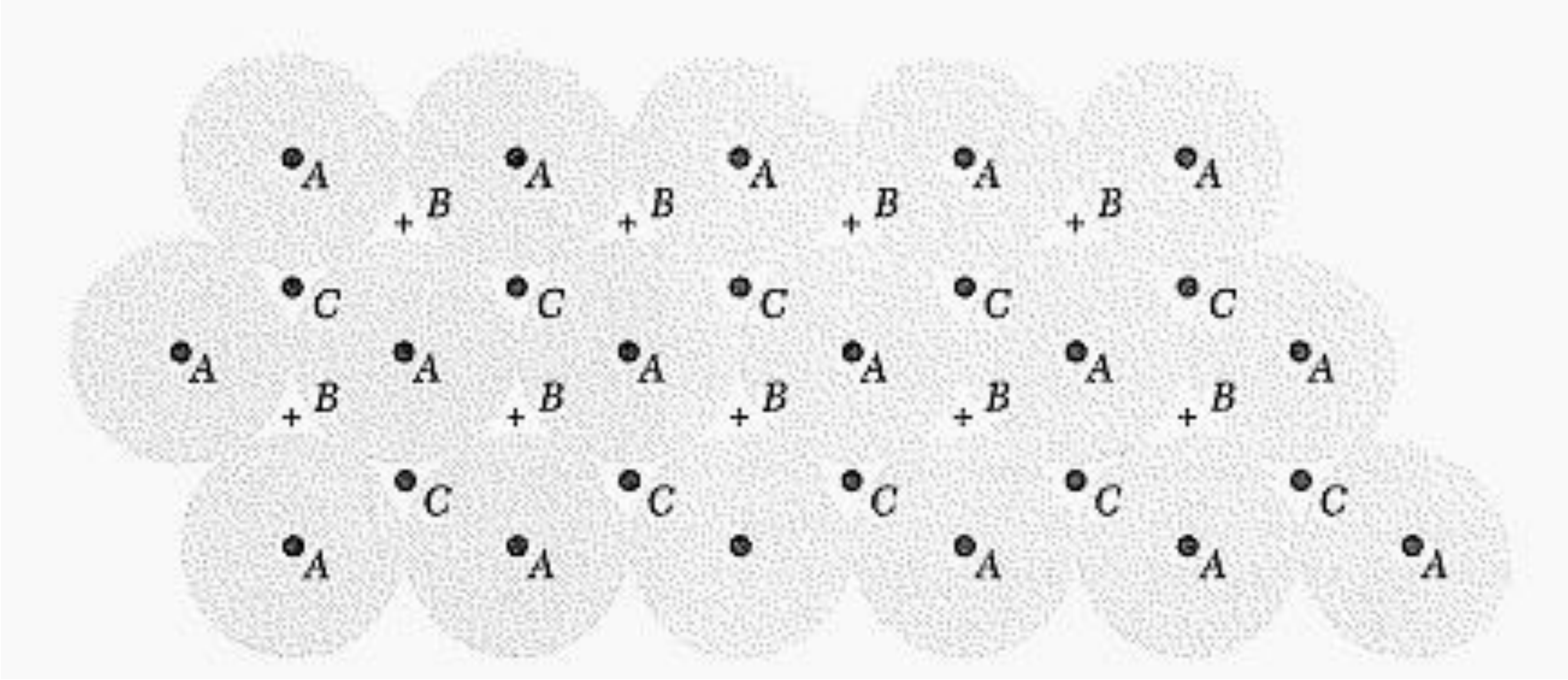


FCC

FOOT & MOUTH VIRUS

BCC

Close-Packed Structures

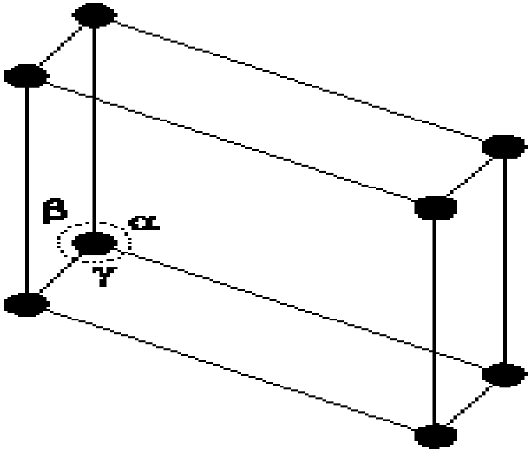


ABCABC… → fcc

ABABAB… → hcp

3 - TRICLINIC & 4 – MONOCLINIC CRYSTAL SYSTEMS

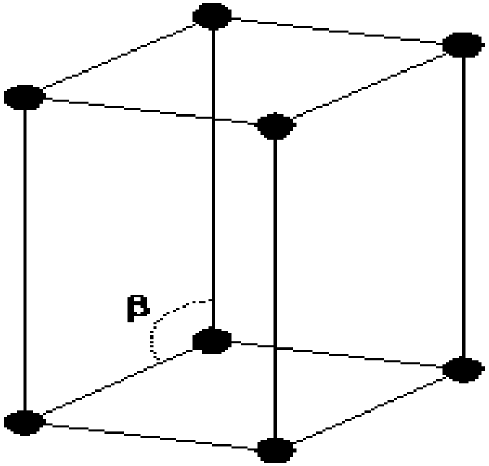
- Triclinic crystals have the least symmetry of any crystal systems. The three axes are each different lengths & none are perpendicular to each other. These materials are the most difficult e.



Triclinic (Simple)

$\alpha \neq \text{ß} \neq \gamma \neq 90^{o}$

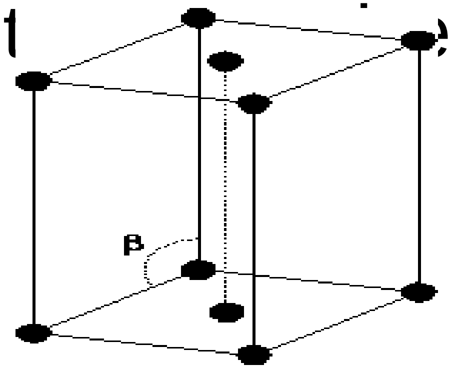
$a \neq b \neq c$



Monoclinic (Simple)

$\alpha = \gamma = 90^{o}, \text{ß} \neq 90^{o}$

$a \neq b \neq c$

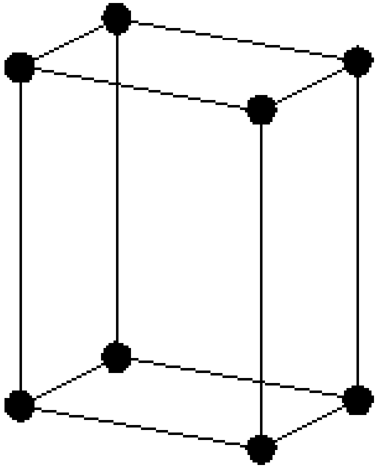


Monoclinic (Base Centered)

$\alpha = \gamma = 90^{o}, \text{ß} \neq 90^{o}$

$a \neq b \neq c$

5 - ORTHORHOMBIC CRYSTAL SYSTEM



Orthorhombic

(Simple)

$\alpha = ß = \gamma = 90^{o}$

$a \neq b \neq c$

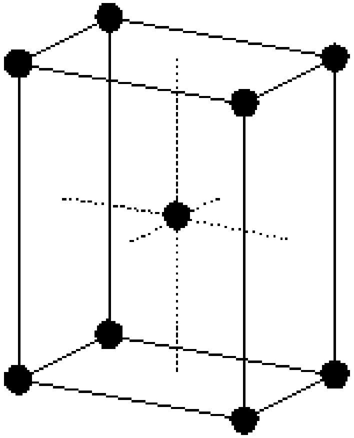
Orthorhombic

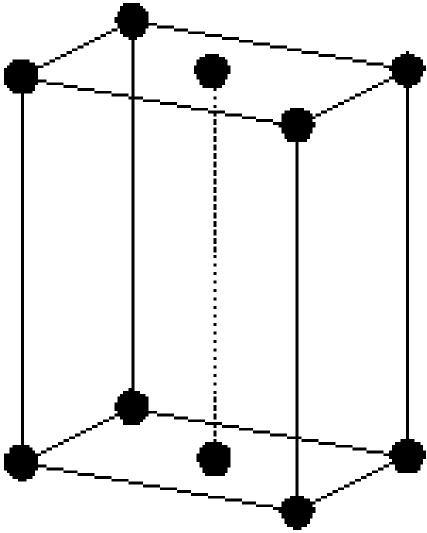
(Body

Centered)

$\alpha = ß = \gamma = 90^{o}$

$a \neq b \neq c$





Orthorhombic

(Base

Centered)

$\alpha = ß = \gamma = 90^{o}$

$a \neq b \neq c$

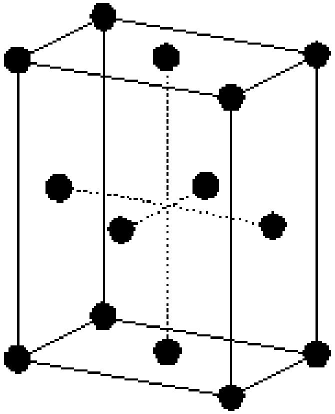
Orthorhombic

(Face

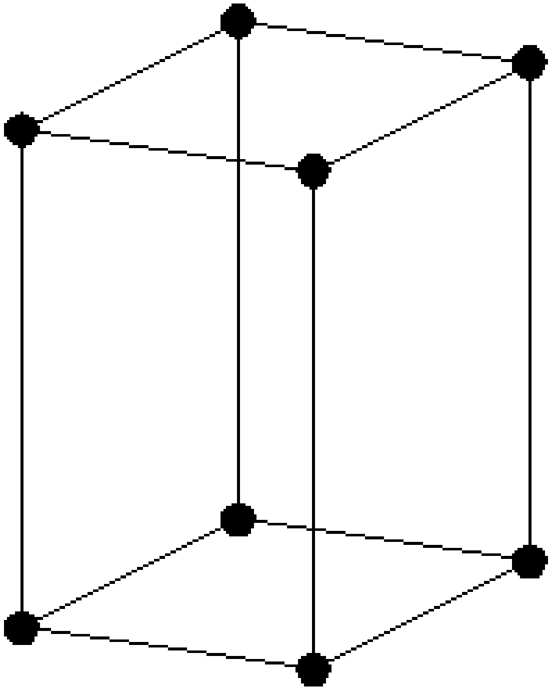
Centered)

$\alpha = ß = \gamma = 90^{o}$

$a \neq b \neq c$



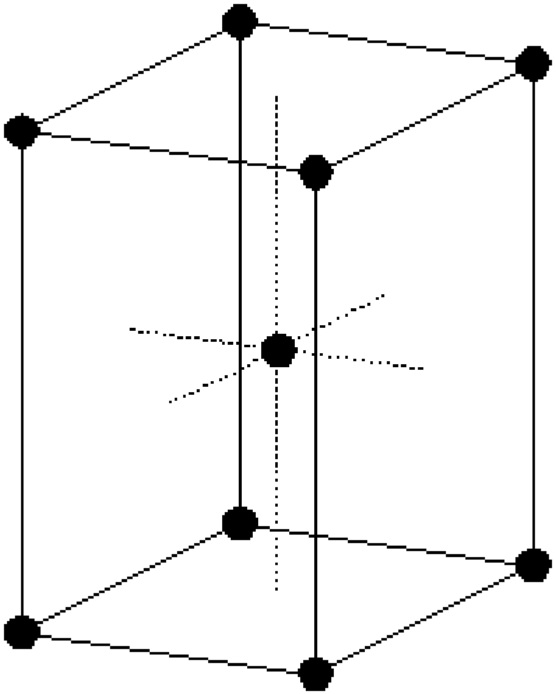
6 – TETRAGONAL CRYSTAL SYSTEM



Tetragonal (P)

$\alpha = \beta = \gamma = 90^{o}$

$a = b \neq c$

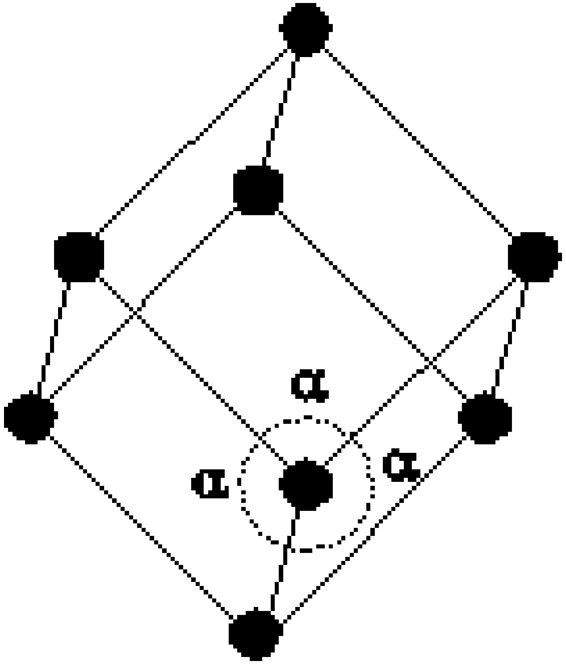


Tetragonal (Body Centered)

$\alpha = \beta = \gamma = 90^{o}$

$a = b \neq c$

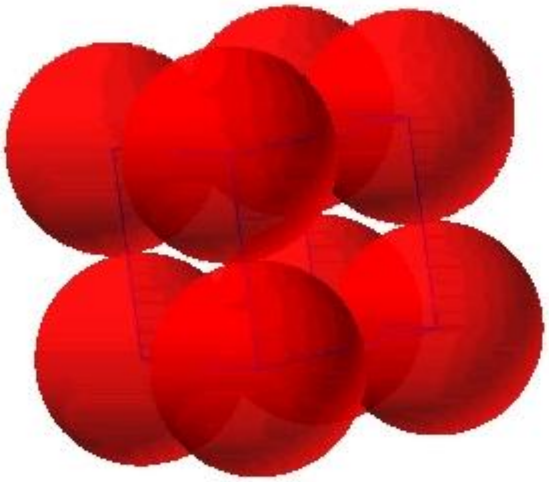
7 - RHOMBOHEDRAL (R) OR TRIGONAL CRYSTAL SYSTEM

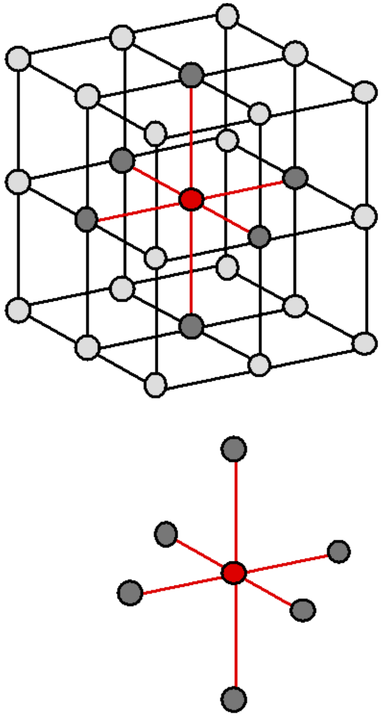


Rhombohedral (R) or
Trigonal (S)
a = b = c, $\alpha = \beta = \gamma \neq 90^{o}$

Simple Cubic Structure (SC)

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





- Coordination No. = 6 (# nearest neighbors) for each atom as seen

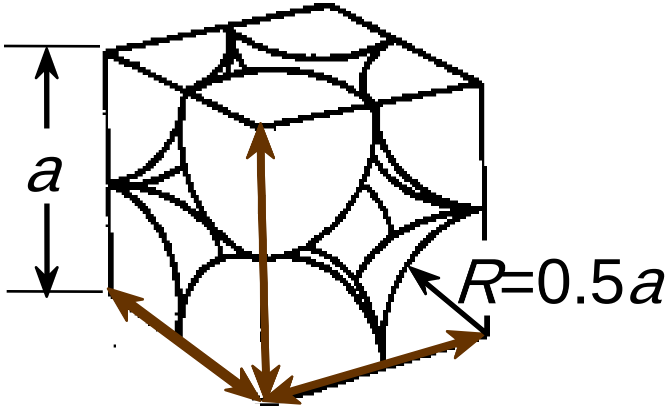
(Courtesy P.M. Anderson)

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



close-packed directions

contains (8 x 1/8) =

1 atom/unit cell

Adapted from Fig. 3.23, *Callister 7e.*

$$\frac{\text{atoms}}{\text{unit cell}} \qquad \frac{\text{volume}}{\text{atom}}$$

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

$$\frac{\text{volume}}{\text{unit cell}}$$

Here: a = R_{at}*2

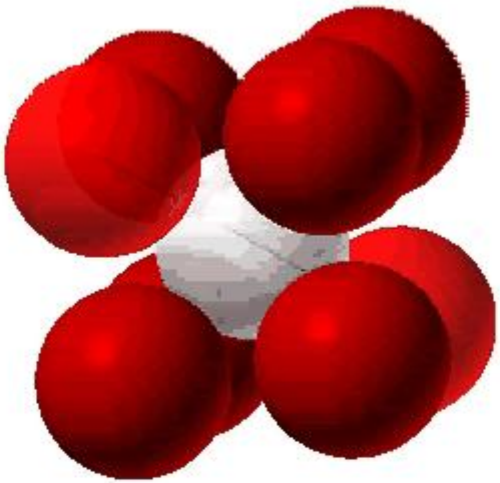
Where R_{at} is the ‘handbook’ atomic radius

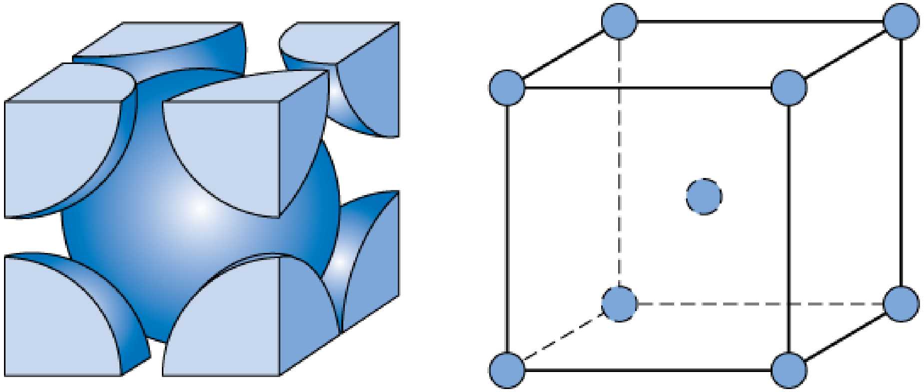
Body Centered Cubic Structure (BCC)

- Atoms touch each other along *cube diagonals within a unit cell*.

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

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





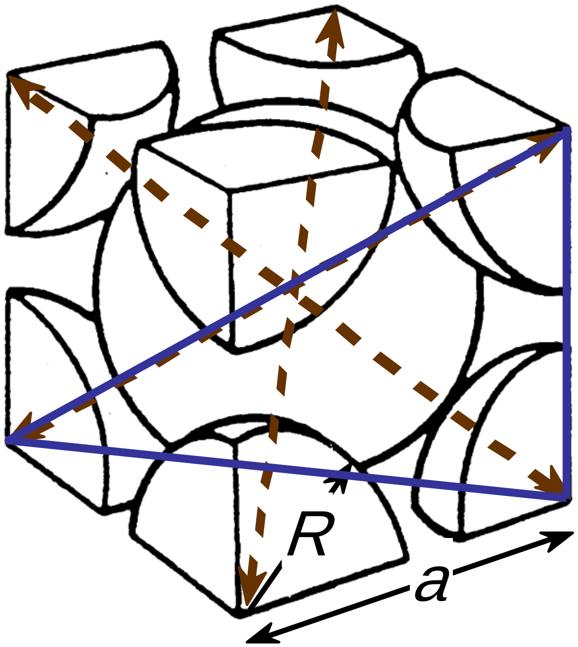
Adapted from Fig. 3.2, *Callister 7e.*

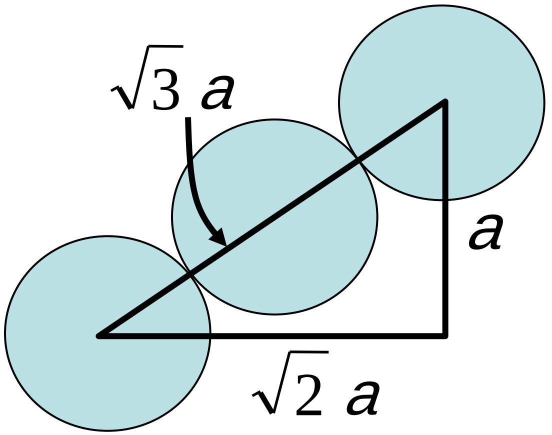
- Coordination # = 8

2 atoms/unit cell: (1 center) + (8 corners x 1/8)

(Courtesy P.M. Anderson)

Atomic Packing Factor: BCC





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

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

$\frac{\text{atoms}}{\text{unit cell}}$ → 2

$\frac{\text{volume}}{\text{atom}}$ → $\frac{4}{3}\pi(\sqrt{3}a/4)^3$

$\frac{\text{volume}}{\text{unit cell}}$ → a^3

Adapted from
Fig. 3.2(a), *Callister 7e.*

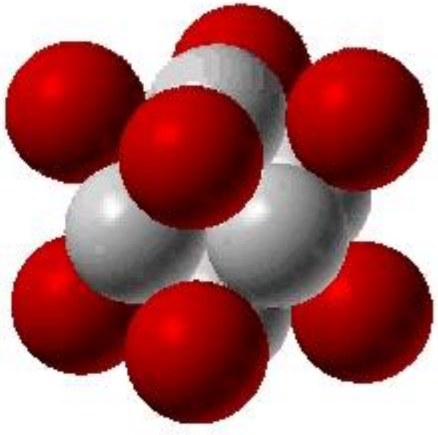
- APF for a body-centered cubic structure = 0.68

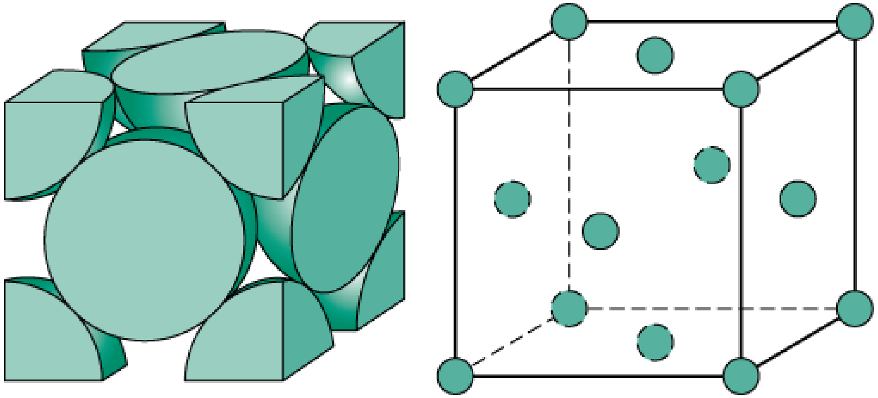
Face Centered Cubic Structure (FCC)

- Atoms touch each other along *face diagonals*.
  - --Note: All atoms are identical; the face-centered atoms are shaded differently only for ease of viewing.

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

- Coordination # = 12





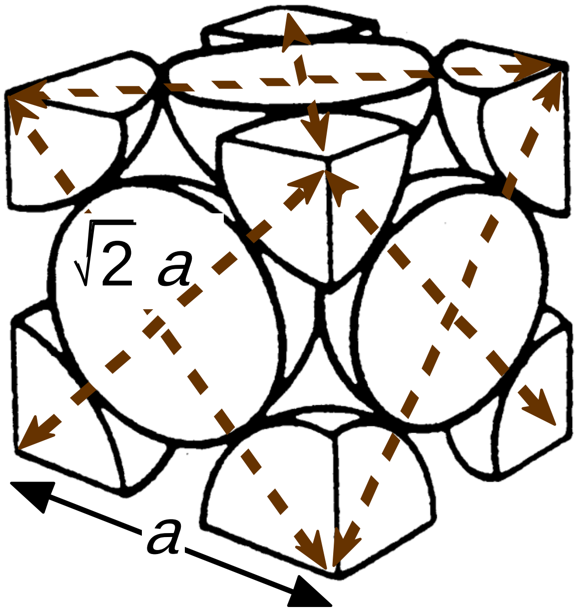
Adapted from Fig. 3.1, *Callister 7e.*

4 atoms/unit cell: (6 face x ½) + (8 corners x 1/8)

(Courtesy P.M. Anderson)

Atomic Packing Factor: FCC

- APF for a face-centered cubic structure = 0.74



Adapted from
Fig. 3.1(a),
Callister 7e.

The maximum achievable APF!

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

(a = 2√2*R)

Unit cell contains:
6 x 1/2 + 8 x 1/8
= 4 atoms/unit cell

$\frac{\text{atoms}}{\text{unit cell}}$

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

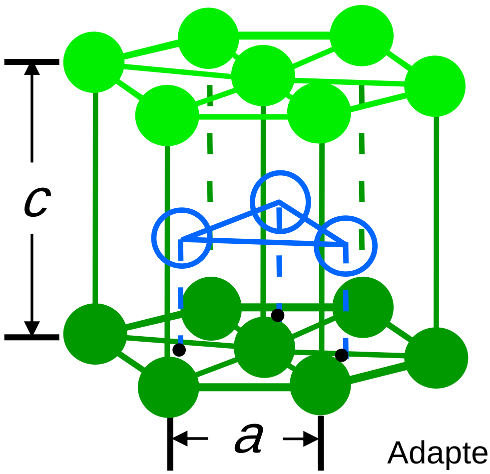
$\frac{\text{volume}}{\text{atom}}$

$\frac{\text{volume}}{\text{unit cell}}$

Hexagonal Close-Packed Structure (HCP)

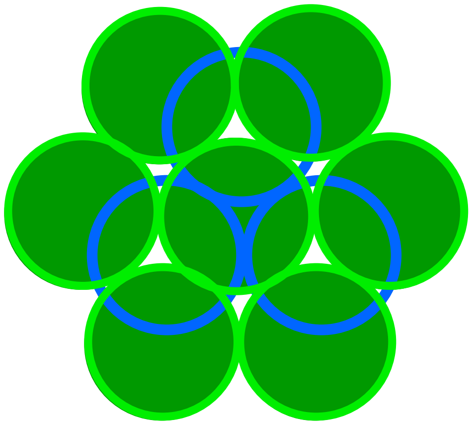
ex: Cd, Mg, Ti, Zn

- ABAB... Stacking Sequence
- 3D Projection



Adapted from Fig. 3.3(a), *Callister 7e.*

- 2D Projection



- Coordination # = 12

6 atoms/unit cell

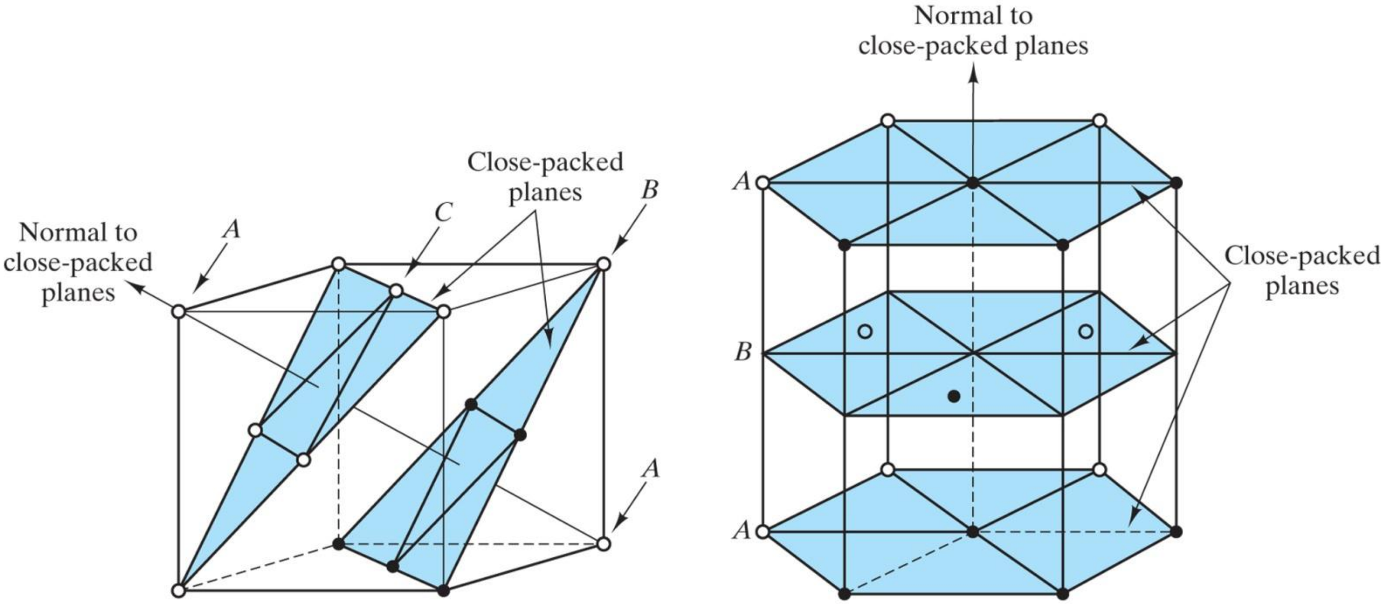
- APF = 0.74

- *c*/*a* = 1.633 *(ideal)*

We find that both FCC & HCP are highest density packing schemes (APF = .74) – this illustration shows their differences as the closest packed planes are "built-up"

(a) Stacking of close-packed planes

(b) Stacking of close-packed planes



(c) Face-centered cubic

(d) Hexagonal close packed

Theoretical Density, ρ

$$\text{Density} = \rho = \frac{\text{Mass of Atoms in Unit Cell}}{\text{Total Volume of Unit Cell}}$$

$$\rho = \frac{nA}{V_C N_A}$$

where

n = number of atoms/unit cell

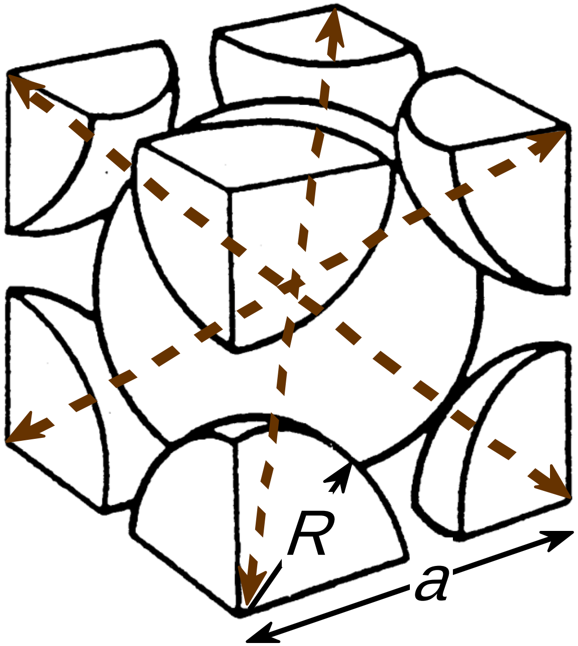
A = atomic weight

V_C = Volume of unit cell = a^3 for cubic

N_A = Avogadro's number

= 6.023×10^{23} atoms/mol

Theoretical Density, ρ



- Ex: Cr (BCC)

  $A = 52.00$ g/mol

  $R = 0.125$ nm

  $n = 2$

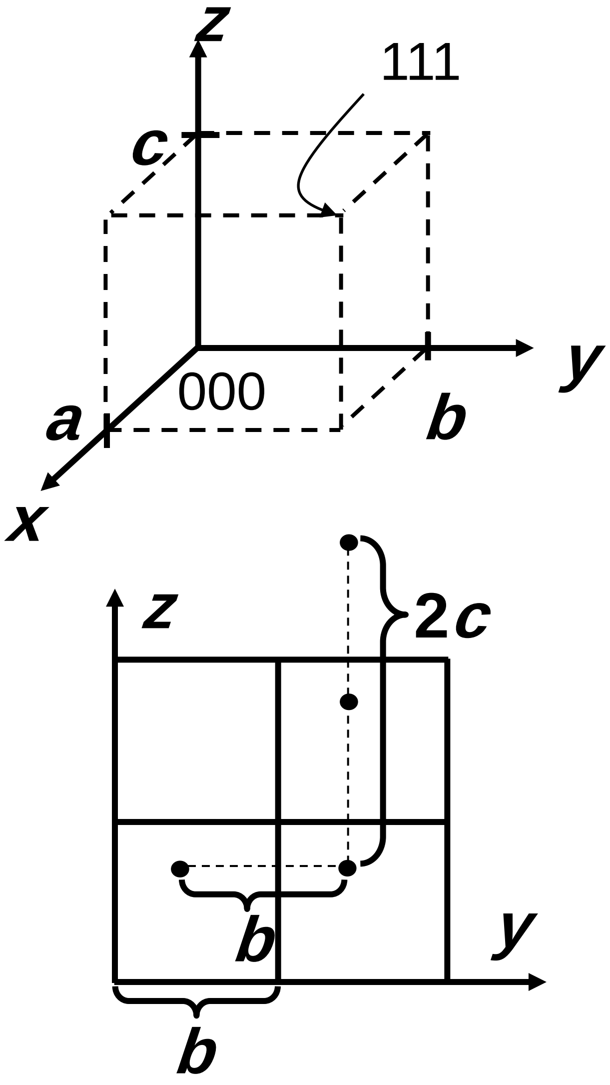
  $\therefore\ a = 4R/\sqrt{3} = 0.2887$ nm

$$\rho = \frac{\overbrace{2}^{\frac{\text{atoms}}{\text{unit cell}}}\ \overbrace{52.00}^{\frac{\text{g}}{\text{mol}}}}{\underbrace{a^3}_{\frac{\text{volume}}{\text{unit cell}}}\ \underbrace{6.023 \times 10^{23}}_{\frac{\text{atoms}}{\text{mol}}}}$$

$\rho_{\text{theoretical}} = 7.18\ \text{g/cm}^3$

$\rho_{\text{actual}} = 7.19\ \text{g/cm}^3$

Locations in Lattices: Point Coordinates



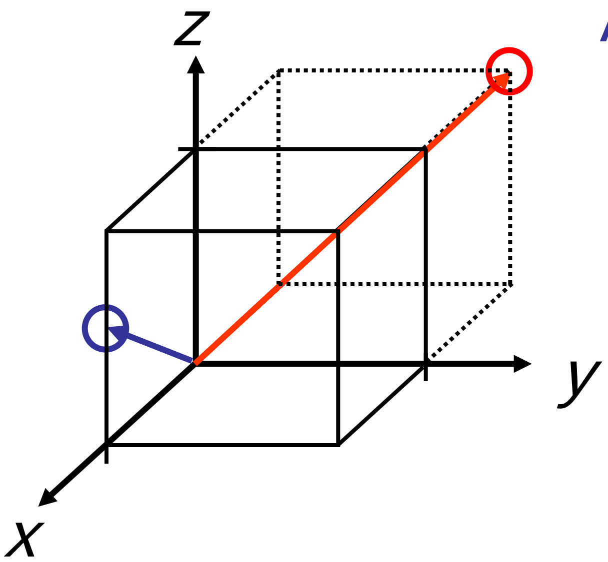
Point coordinates for unit cell center are

a/2, *b*/2, *c*/2 ½½½

Point coordinates for unit cell (body diagonal) corner are 111

Translation: integer multiple of lattice constants → identical position *in another unit cell*

Crystallographic Directions



Algorithm

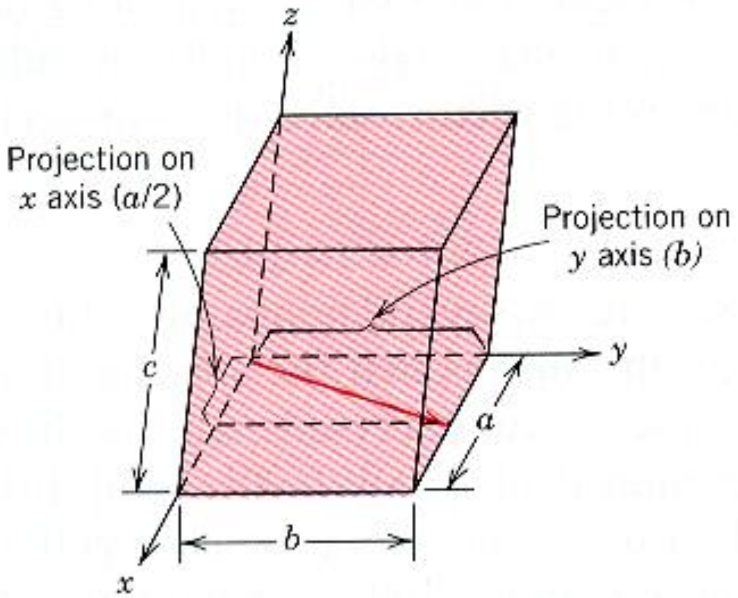
1. Vector is repositioned (if necessary) to ***pass through the Unit Cell origin***.
2. Read off line projections (to principal axes of U.C.) in terms of unit cell dimensions *a*, *b*, and *c*
3. Adjust to smallest **integer values**
4. Enclose in square brackets, *no commas*

[*uvw*]

ex: 1, 0, ½ => 2, 0, 1 => [201]

-1, 1, 1 => $[\bar{1}11]$ where 'overbar' represents a negative index

families of directions <*uvw*>

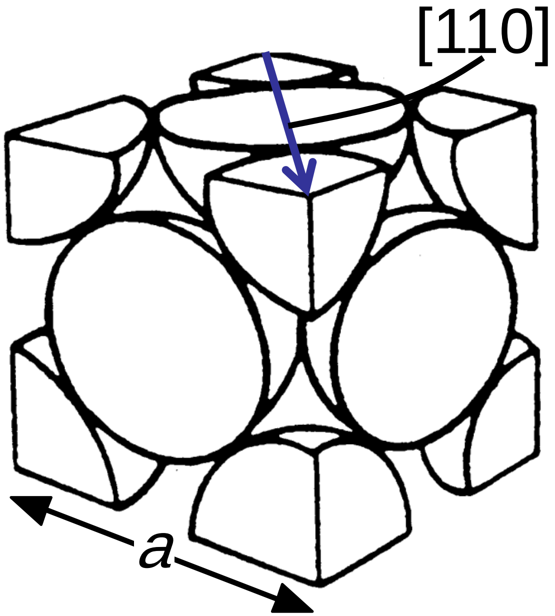


What is this ***Direction ?????***

	x	*y*	*z*
Projections:	a/2	b	0c
Projections in terms of a,b and c:	1/2	1	0
Reduction:	1	2	0
Enclosure [brackets]		**[120]**	

Linear Density – considers equivalance and is important in Slip

- Linear Density of Atoms ≡ LD = $\dfrac{\text{Number of atoms}}{\text{Unit length of direction vector}}$



ex: linear density of Al in [110] direction

$a = 0.405$ nm

atoms

$$\text{LD} = \frac{2}{\sqrt{2}a} = \boxed{3.5\ \text{nm}^{-1}}$$

length

atoms **CENTERED** on the direction of interest!

Length is of the **direction** of interest **within** the Unit Cell

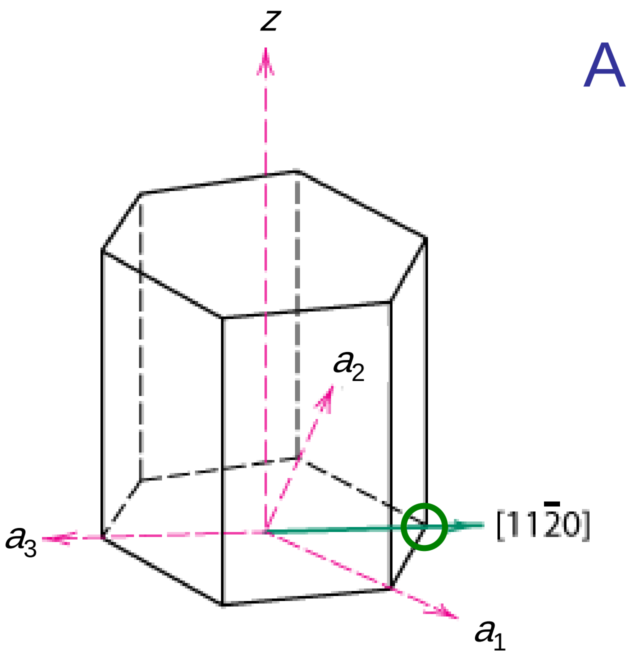
Determining Angles Between Crystallographic Direction:

$$\theta = Cos^{-1}\left[\frac{u_1u_2 + v_1v_2 + w_1w_2}{\sqrt{\left(u_1^2 + v_1^2 + w_1^2\right)\bullet\left(u_2^2 + v_2^2 + w_2^2\right)}}\right]$$

Where u_i's , v_i's & w_i's are the “Miller Indices” of the directions in question

– also (for information) If a direction has the same Miller Indices as a plane, it is NORMAL to that plane

HCP Crystallographic Directions



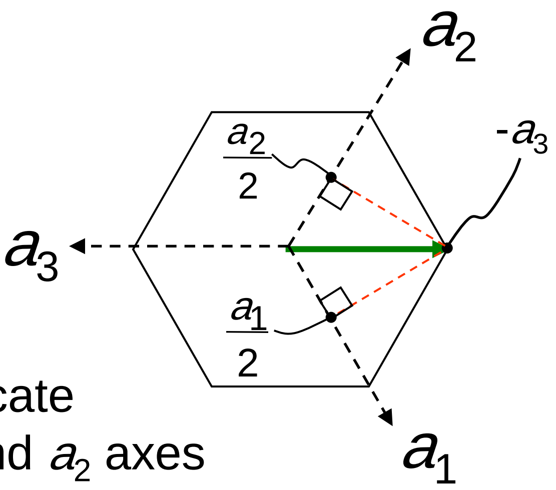
Adapted from Fig. 3.8(a), *Callister 7e.*

Algorithm

1. Vector repositioned (if necessary) to pass through origin.
2. Read off projections in terms of unit cell dimensions a_1, a_2, a_3, or c
3. Adjust to smallest integer values
4. Enclose in square brackets, no commas

$[uvtw]$

ex: ½, ½, -1, 0 => $[11\bar{2}0]$



dashed red lines indicate projections onto a_1 and a_2 axes

HCP Crystallographic Directions

- <u>Hexagonal Crystals</u>
  - 4 parameter Miller-Bravais lattice coordinates are related to the direction indices (i.e., $u'v'w'$) in the '3 space' Bravais lattice as follows.

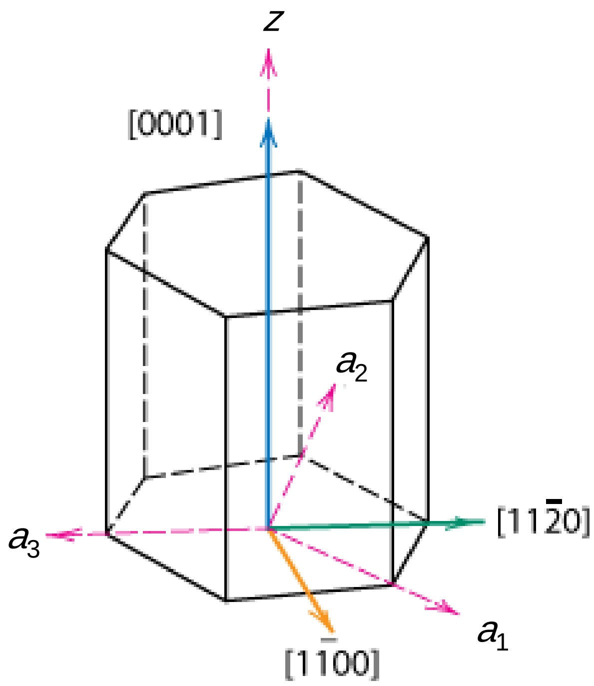


Fig. 3.8(a), *Callister 7e.*

$$[u'v'w'] \rightarrow [uvtw]$$

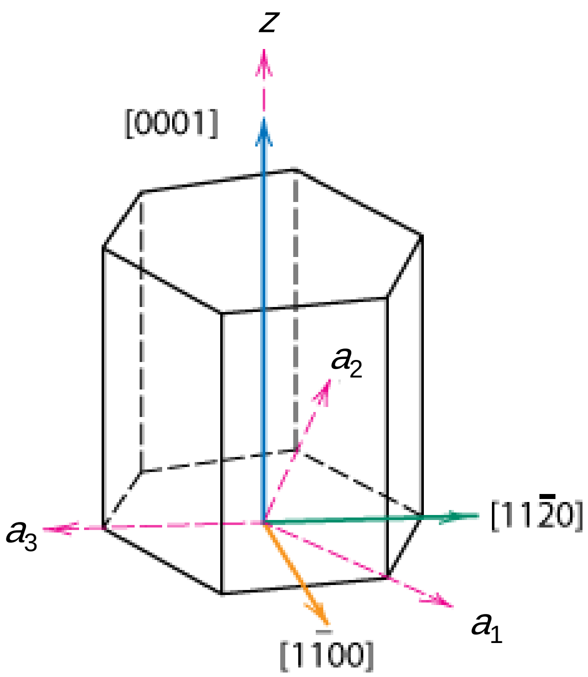
$$u = \frac{1}{3}(2u' - v')$$

$$v = \frac{1}{3}(2v' - u')$$

$$t = -(u + v)$$

$$w = w'$$

Computing HCP Miller- Bravais Directional Indices (an alternative way):



We confine ourselves to the bravais parallelopiped in the hexagon: a_1-a_2-Z and determine: (u’,v’w’)

Here: [1 1 0] - so now apply the models to create M-B Indices

$$u = \tfrac{1}{3}\left(2u' - v'\right) = \tfrac{1}{3}\left(2*1-1\right) = \tfrac{1}{3} \rightarrow 1$$

$$v = \tfrac{1}{3}\left(2v' - u'\right) = \tfrac{1}{3}\left(2*1-1\right) = \tfrac{1}{3} \rightarrow 1$$

$$t = -\left(u+v\right) = -\left(\tfrac{1}{3} + \tfrac{1}{3}\right) = -\tfrac{2}{3} \rightarrow -2$$

$$w = w' = 0$$

M-B Indices: $[11\bar{2}0]$

- Similarly, the distance between any two successive lattice points along the Y-direction is taken as `b’.
- Here $\vec{a}$ and $\vec{b}$ are said to be lattice translational vectors. Consider a square lattice in which $\vec{a}=\vec{b}$.