Introduction to Solid State Physics

Introduction

- Why do materials vary in their properties?

- Because they have different chemical composition.
- Atoms in solid material are arranged in certain special ways.
- The way in which the atoms and molecules arranged has effect on its properties.
- The properties that affected by structure can be termed as Structure sensitive properties.

Structure sensitive and insensitive properties

Structure sensitive	Structure insensitive
Mechanical strength	Melting point
Ductility	Specific heat
Thermal conductivity	Heat of fusion
Electric conductivity	Electrochemical potential

Type of materials

- Metals: are composed of elemental atoms and have such general properties such as easy shaping, good thermal and electrical conductivities.

(examples: iron, copper, Aluminum, Zinc,……..)

Type of materials

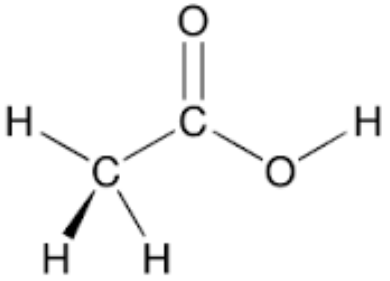
- Ceramics : are solid inorganic compound.
- They are generally hard but easily broken, bad conductor of heat and electricity and possesses high melting points
- Some are good conductors and superconductors

(examples: glass, porcelain, MgO, NaCl, ZnS……)

Type of materials

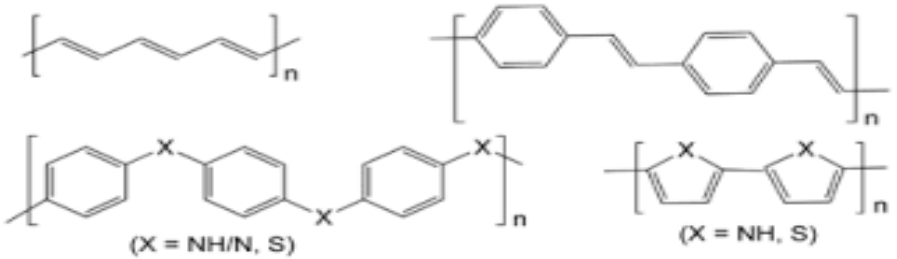
- Organic materials: consists of two types

1- small molecule organic materials



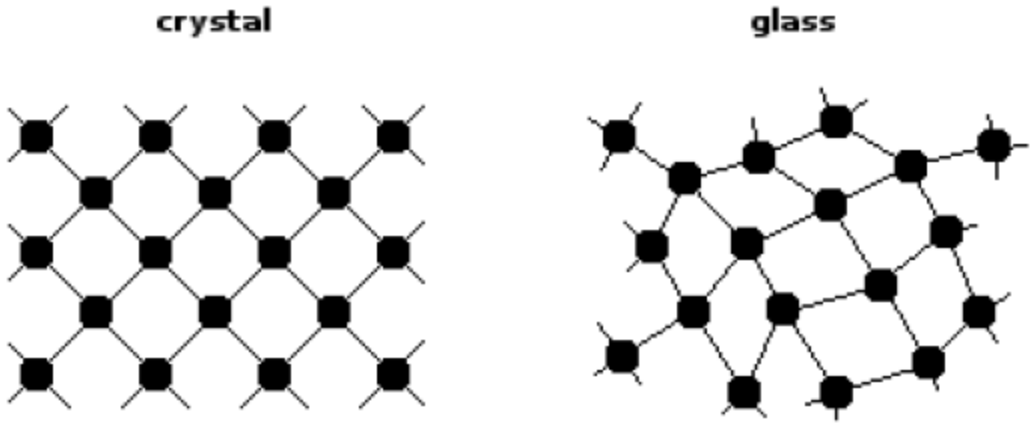
2- large molecule organic materials (Polymers) are composed of large molecular weight organic solids that are generally light in weight, good insulator of heat and electricity and are generally weak mechanically.

(examples: Plastics, rubber, PVC, PVA, PAN, PANI,.....)

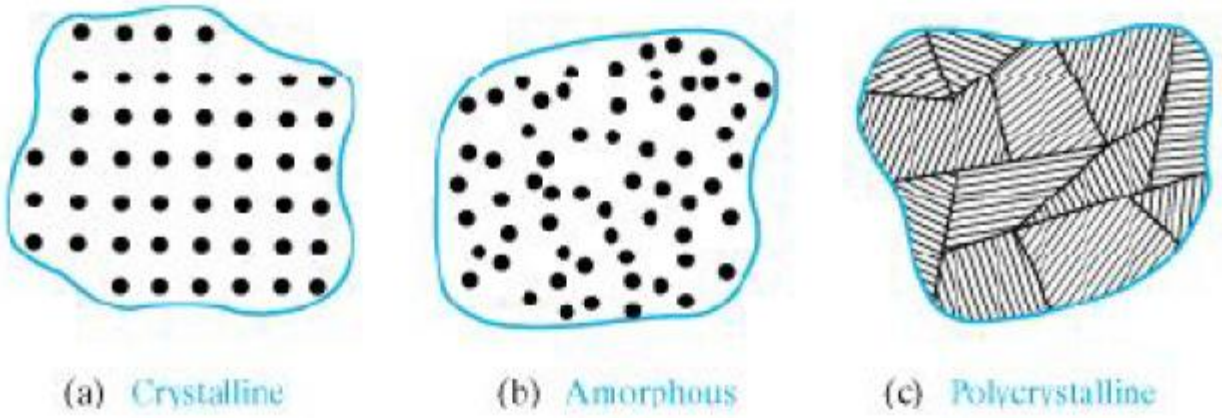


Crystalline Solids

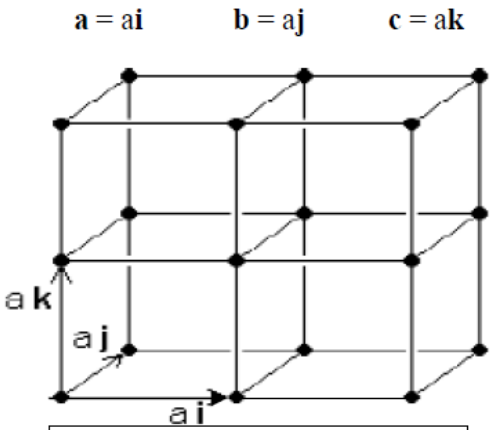
- In crystalline solids, atoms in a solid tends to arrange themselves in orderly regular patterns, in which each atom has the same surroundings i.e. has the same number of neighbors distributed in the same direction in space.
- Crystalline solids are thus defined as a solids in which atoms are arranged in long range order
- Amorphous materials *or glasses are short range order materials.*



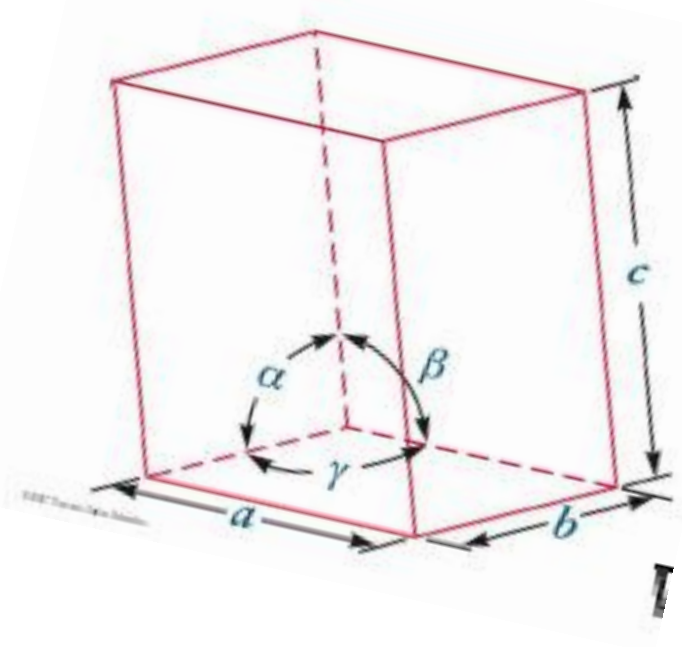
الشكل(4):البنية البلورية(crystal)والبنية الزجاجية(glass)



The unit cell



الشكل (10):البناء البلوري لشبكة مكعبة

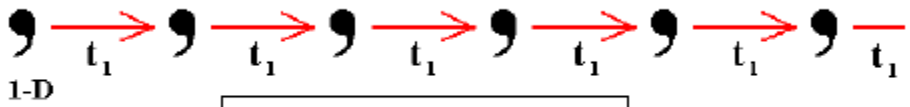


* The unit cell is the smallest basic volume of a crystal
*The unit cell is defined by its shape and its dimensions.
*The unit cell dimensions are called lattice parameters
*The lattice parameters are the edge lengths (a, b and c) and the angels (α, β and γ)

Crystal structure

Bravais lattices in one dimensions **الشبكات الخطية**

لها هيكل مرتب خطيا وهي عبارة عن عقد مرتبة بانتظام في بعد واحد (على طول خط مستقيم) يستفاد من هذه الشبكات للدراسات البسيطة والمبدئية لفهم الحالة الصلبة مثل ذبذبة الشبكات في حالة البعد الواحد



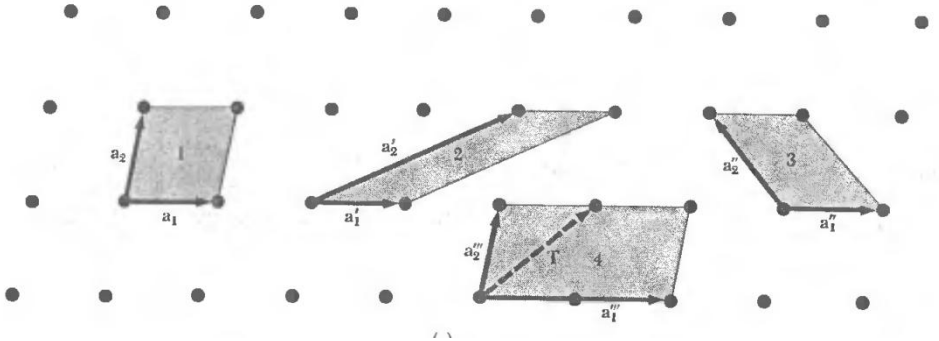
الشكل(1): شبكة خطية

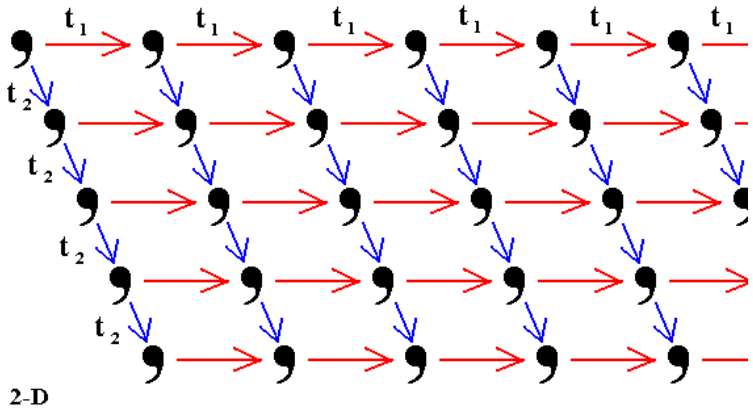
Crystal structure

Bravais lattices in two dimensions

الشبكات ثنائية البعد(شبكات برافيس المستوية)

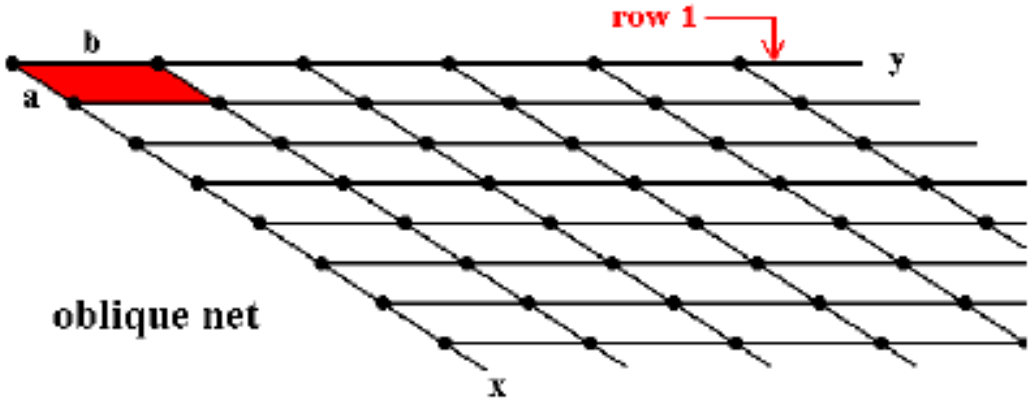
وهي ترتيب لعقد الشبكة البلورية في وتكون على هيئة ترتيب منتظم بشكل خارطة ممتدة بواسطة متجهتين





الشبكات ثنائية البعد(شبكات برافيس المستوية

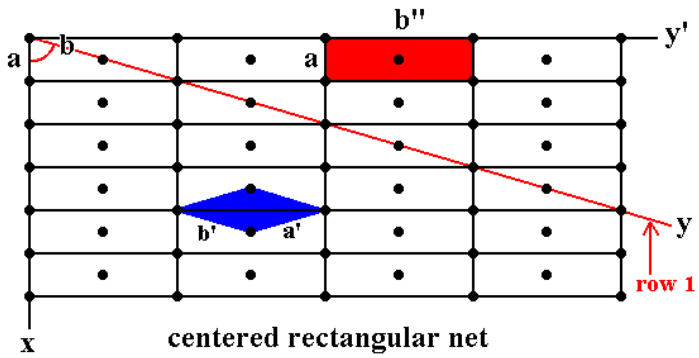
(the *oblique lattice)* الشكل العام للشبكة المستوية هو المسمى بالشبكة المائلة

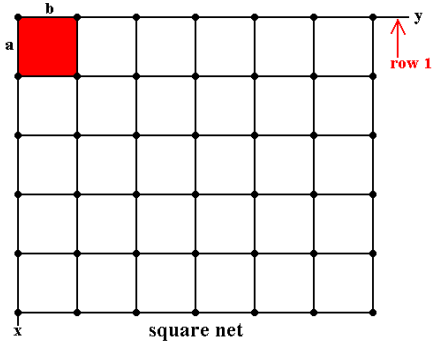


الشبكات ثنائية البعد(شبكات برافيس المستوية

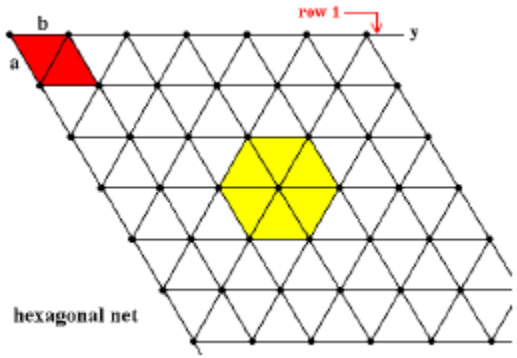
يوجد بالإضافة إلى الشبكة المائلة أربع أنواع من الشبكات المستوية هي

المستطيلة و المستطيلة المركزية

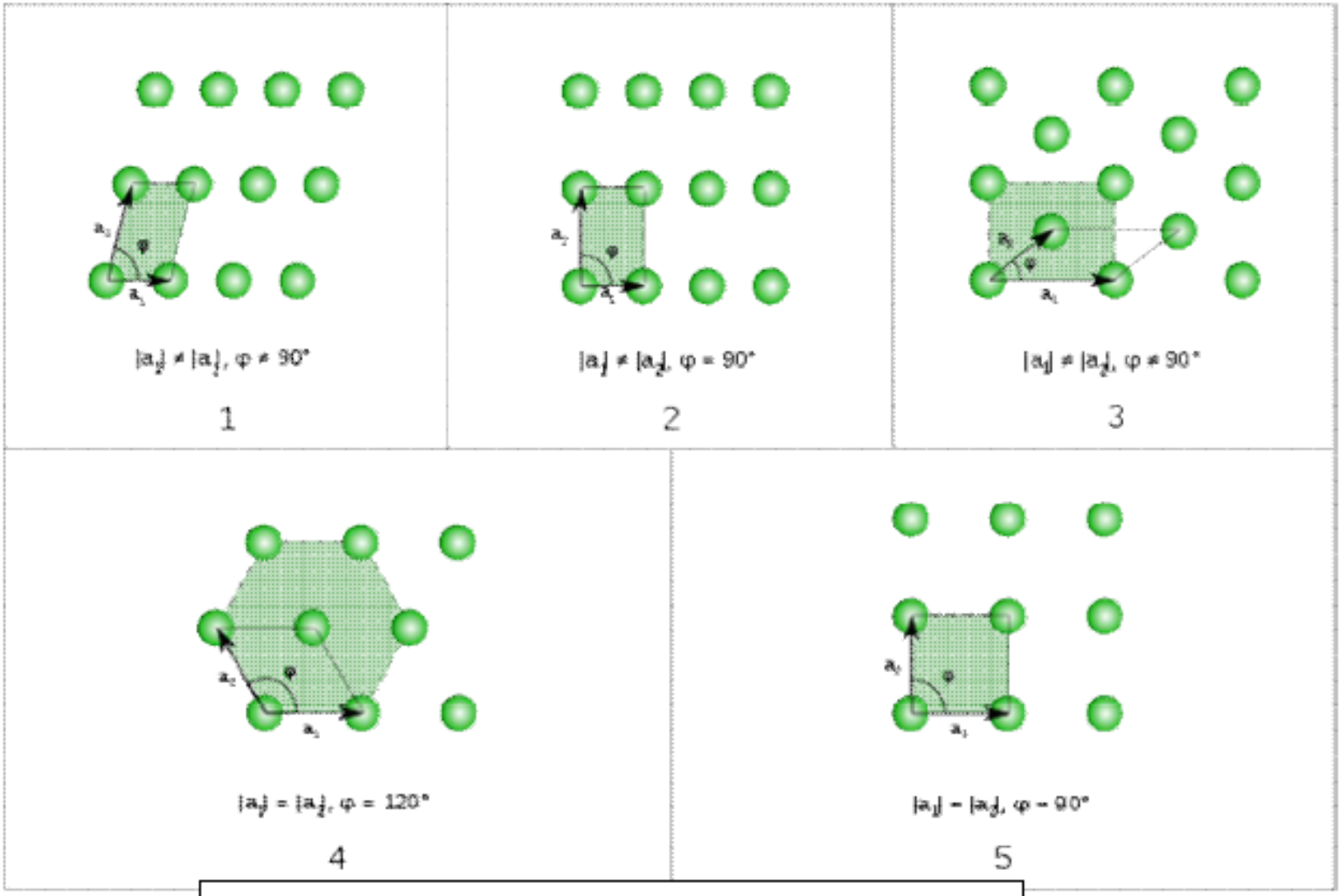




المربعة



والسداسية

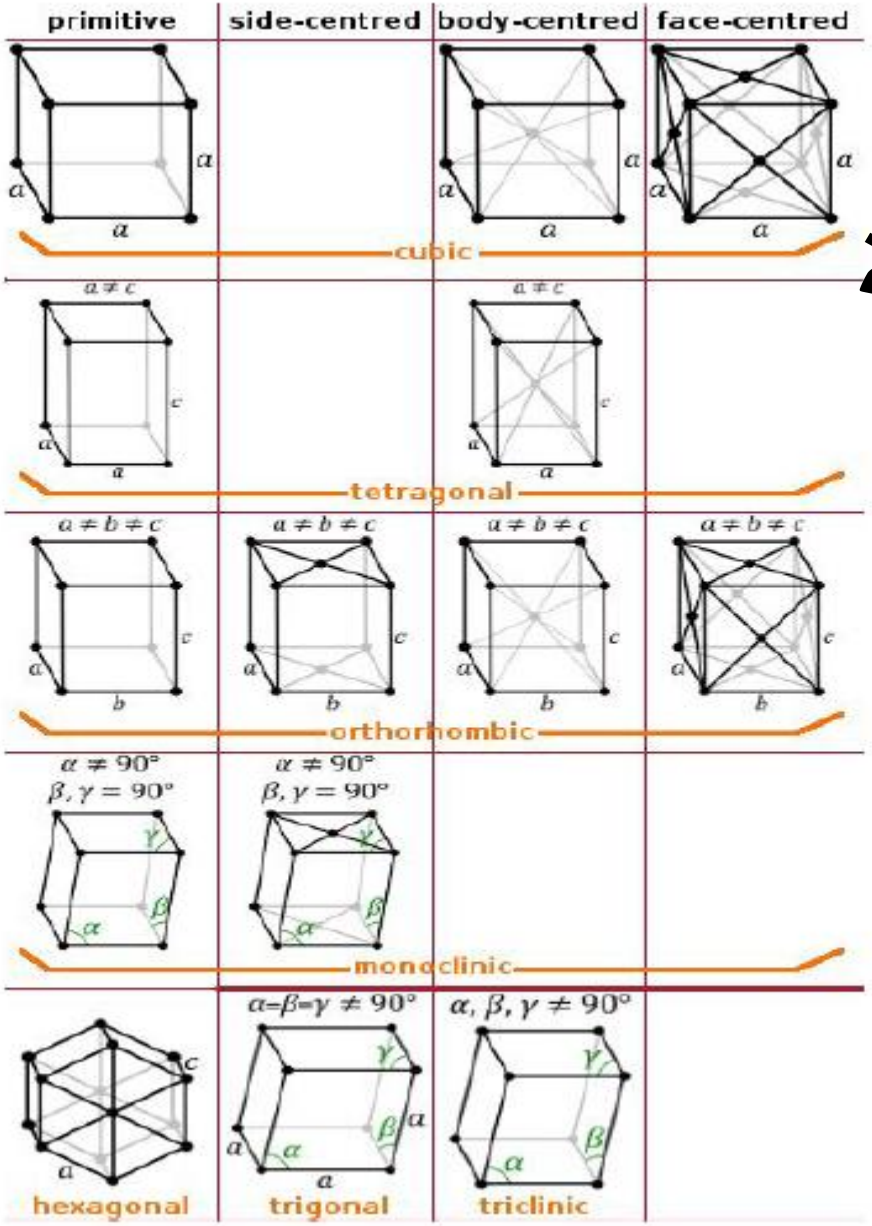


الشكل(5): شكل آخر للشبكات المستوية الخمسة

Bravais lattices in three dimensions

شبكات برافيس ثلاثية الأبعاد

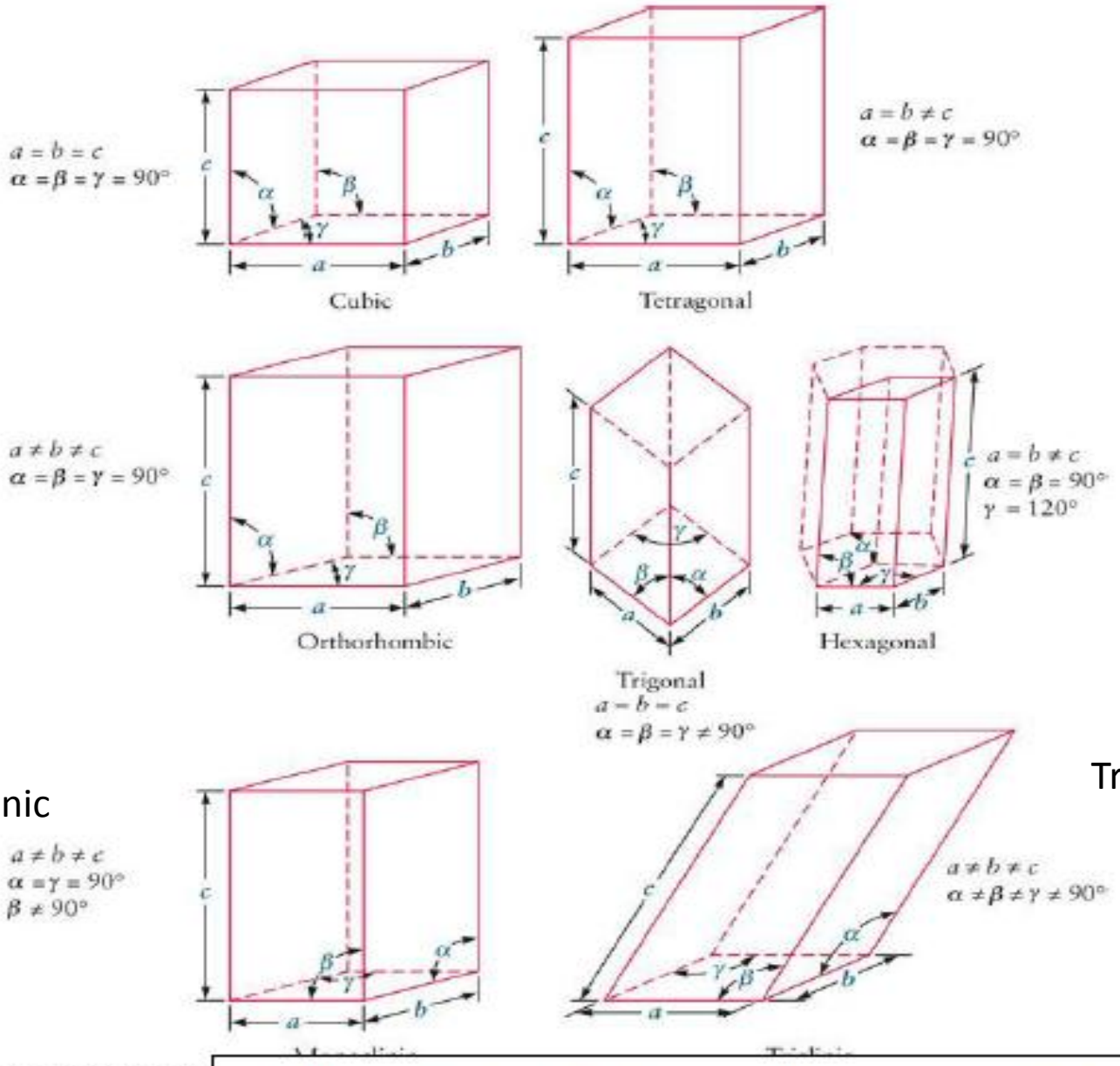
1. ثلاثية الميل (triclinic) ولها شكل بسيط مثل($CuSO_4,5H_2O$).
2. أحادية الميل (monoclinic)ولها **شكلين بسيط ومركزي القاعدة** مثل(Na_2CO_3).
3. المعينية (orthorhombic) ولها **أربعة أشكال** بسيط,مركزي القاعدة,مركزي متوازي السطوح,مركزي الوجوه مثل ($AgNO_3$).
4. الرباعية (tetragonal) ولها **شكلين** بسيط ومركزية متوازية السطوح مثل (KH_2PO_4).
5. ثلاثية متساوية الأحرف (trigonal) ولها **شكل واحد** (شبه معينية بسيطة) مثل($CuCO_3$).
6. السداسية (hexagonal) ولها **شكل واحد** مثل(Zn,SiO_2).
7. المكعبة (cubic) ولها **ثلاثة أشكال مهمة جدا** وهي المكعبة البسيطة((simple cubic(SC))مثل (Na,K,Li) ثم المكعبة المركزية وتعني وجود ذرة في مركز المكعب((Body-Centered Cubic(BCC))مثل (Fe,Cr,v,Ba)ثم المكعبة مركزية الوجوه((Face-Centered Cubic(FCC)) مثل (Al,Cu,Ag,Au).



Bravais lattices in three dimensions

شبكات برافيس ثلاثية الأبعاد

تصنف الشبكات الأربعة عشر في سبعة أصناف رئيسية



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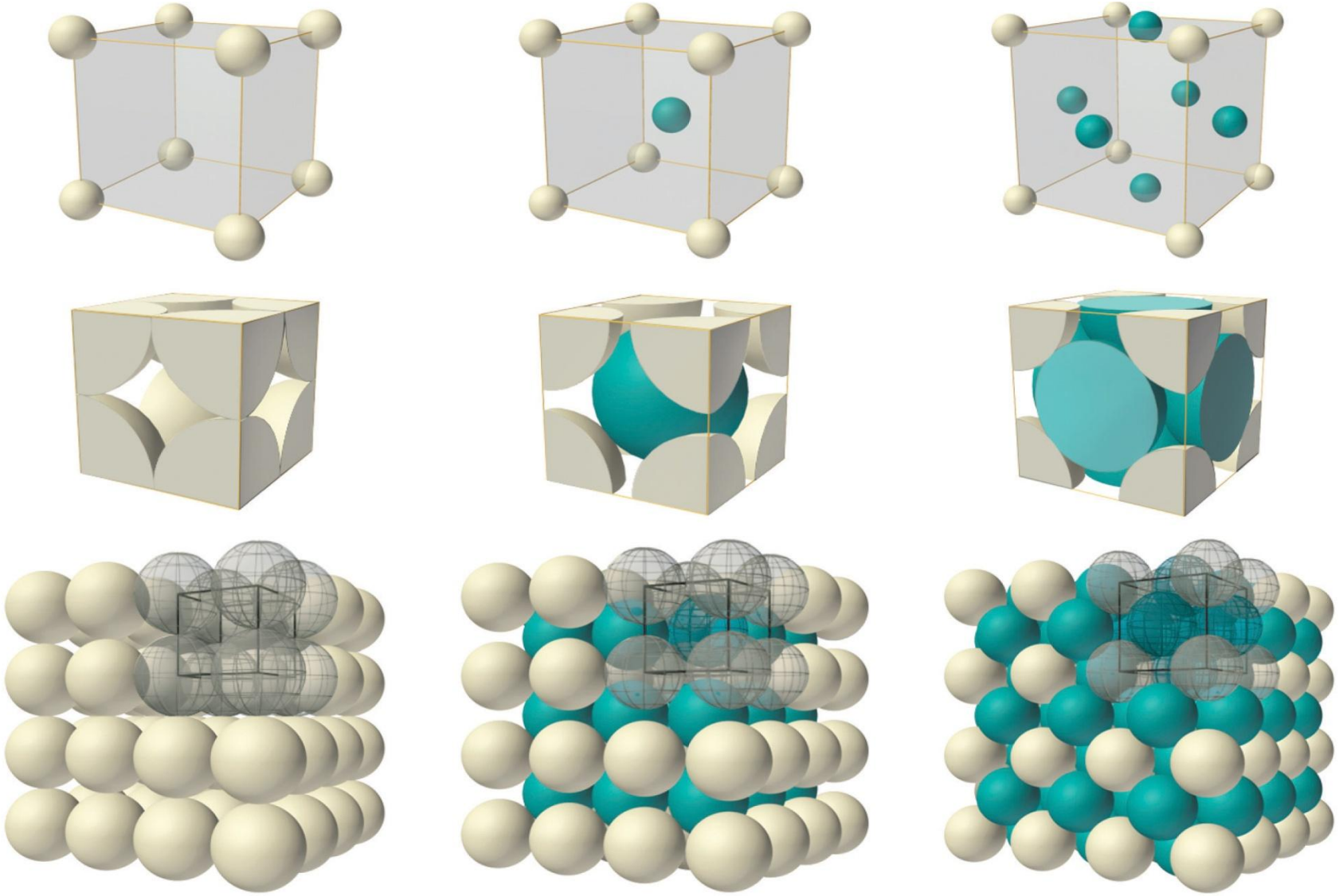
الشكل (8): التصنيف السباعي لشبكات برافيس الثلاثية

Metallic crystals

- Elements of groups I, II, III of the periodic table together with the transitional elements are metals.
- In a metallic bond the valence electrons are bonded loosely to their atoms and are free to move.
- All metals, when prepared in the normal ways are crystalline.
- In a metallic crystal, an atom would try to surround itself with the maximum possible number of neighbors in order to minimize the bond energy per unit volume.
- Metals are expected to crystallize in structures with the densest packing of atoms.

Cubic structures



(a) Simple cubic

(b) Body-centered cubic

(c) Face-centered cubic

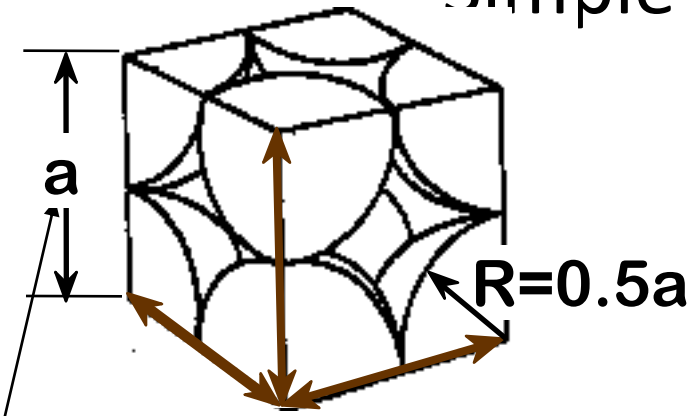
Atomic packing factor

- In crystallography, **atomic packing factor** (APF) or **packing fraction** is the fraction of volume in a crystal structure that is occupied by atoms. It is dimensionless and always less than unity. For one-component crystals (those that contain only one type of atom), the APF is represented mathematically by

$$APF = \frac{N_{atoms} \times V_{atom}}{V_{unit\ cell}} = \frac{Volume\ of\ Atoms\ in\ Unit\ Cell}{Volume\ of\ Unit\ Cell}$$

- where N_{atoms} is the number of atoms in the crystal, V_{atom} is the volume of an atom, and $V_{crystal}$ is the volume occupied by the crystal. It can be proven mathematically that for one-component structures.
- The most dense arrangement of atoms has an APF of about 0.74. In reality, this number can be higher due to specific intermolecular factors.
- For multiple-component structures, the APF can exceed 0.74.

ATOMIC PACKING FACTOR
Simple cubic structure (SC)



Adapted from Fig. 3.19, *Callister 6e.*

Lattice constant

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

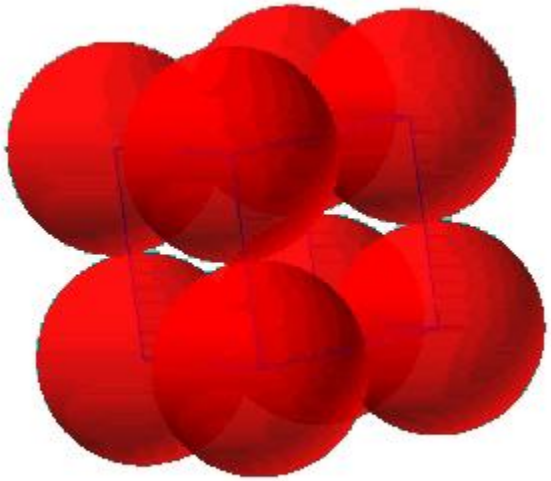
$$APF = \frac{\text{atoms}}{\text{unit cell}} \cdot \frac{\text{volume}}{\text{atom}} \Big/ \frac{\text{volume}}{\text{unit cell}} = \frac{1 \cdot \frac{4}{3}\pi (0.5a)^3}{a^3}$$

- APF for a simple cubic structure = 0.52

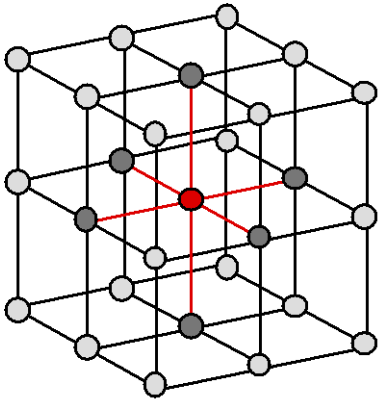
SIMPLE CUBIC STRUCTURE (SC)

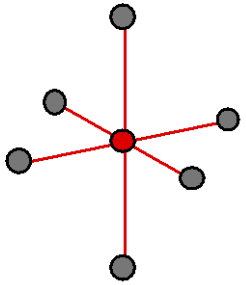
- Cubic unit cell is 3D repeat unit
- Close-packed directions (directions along which atoms touch each other) are cube edges.

- **Coordination # = 6**
(# nearest neighbors)

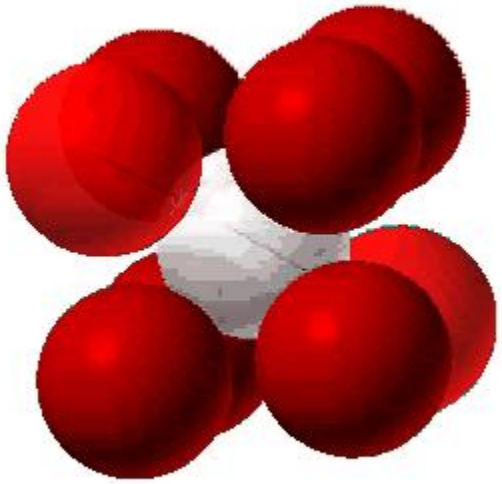


(Courtesy P.M. Anderson)



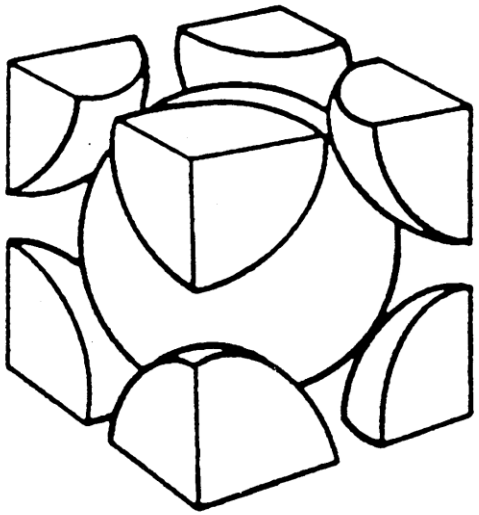


BODY CENTERED CUBIC STRUCTURE (BCC)



(Courtesy P.M. Anderson)

- Coordination # = 8

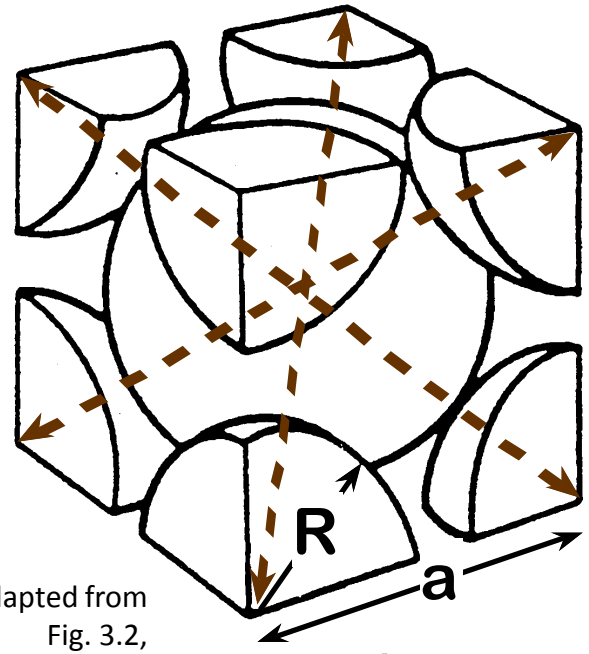


Adapted from Fig. 3.2, *Callister 6e.*

- Close packed directions are cube diagonals.

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

ATOMIC PACKING FACTOR: BCC



Adapted from Fig. 3.2, *Callister 6e.*

Close-packed directions:

length = 4R

$= \sqrt{3}\, a$

Number of atoms per unit cell= 1+8x(1/8)

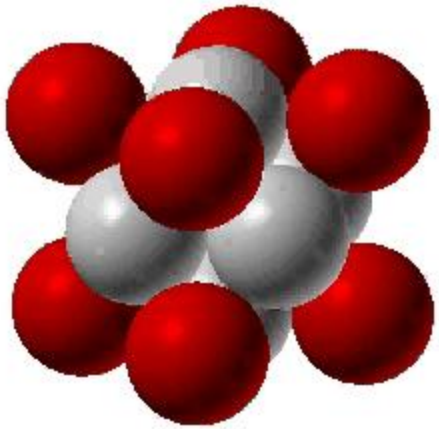
= 2 atoms/unit cell

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

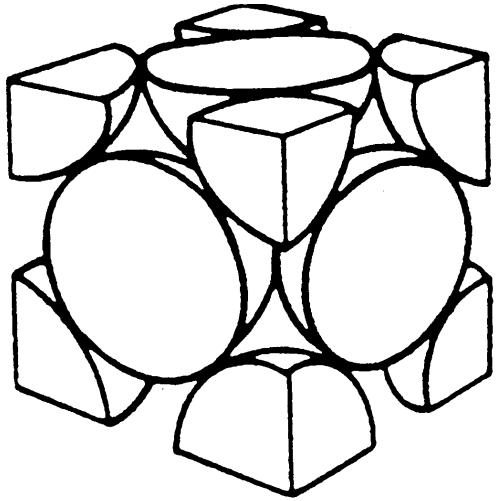
- APF for a body-centered cubic structure = $\pi\sqrt{3}/8 = 0.68$

FACE CENTERED CUBIC STRUCTURE (FCC)

- Coordination # = 12



(Courtesy P.M. Anderson)

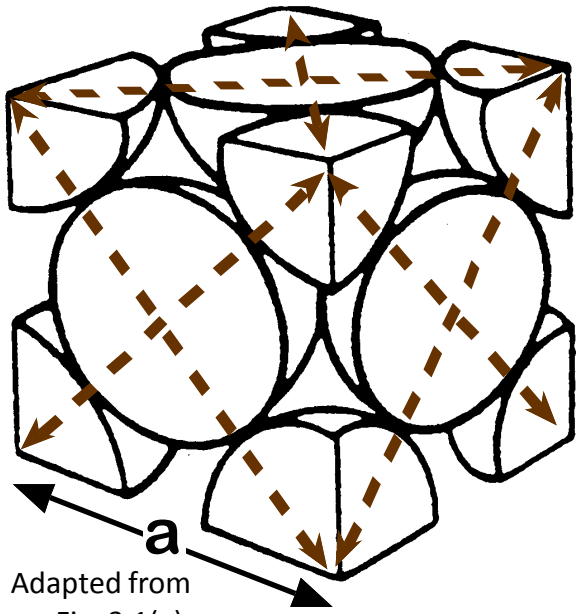


Adapted from Fig. 3.1(a), *Callister 6e.*

- Close packed directions are face diagonals.

  --Note: All atoms are identical; the face-centered atoms are shaded differently only for ease of viewing.

ATOMIC PACKING FACTOR: FCC



Adapted from Fig. 3.1(a), *Callister 6e.*

Close-packed directions:

length = 4R

$= \sqrt{2}\, a$

Number of atoms per unit cell= 6x(1/2)+8x(1/8)

= 4 atoms/unit cell

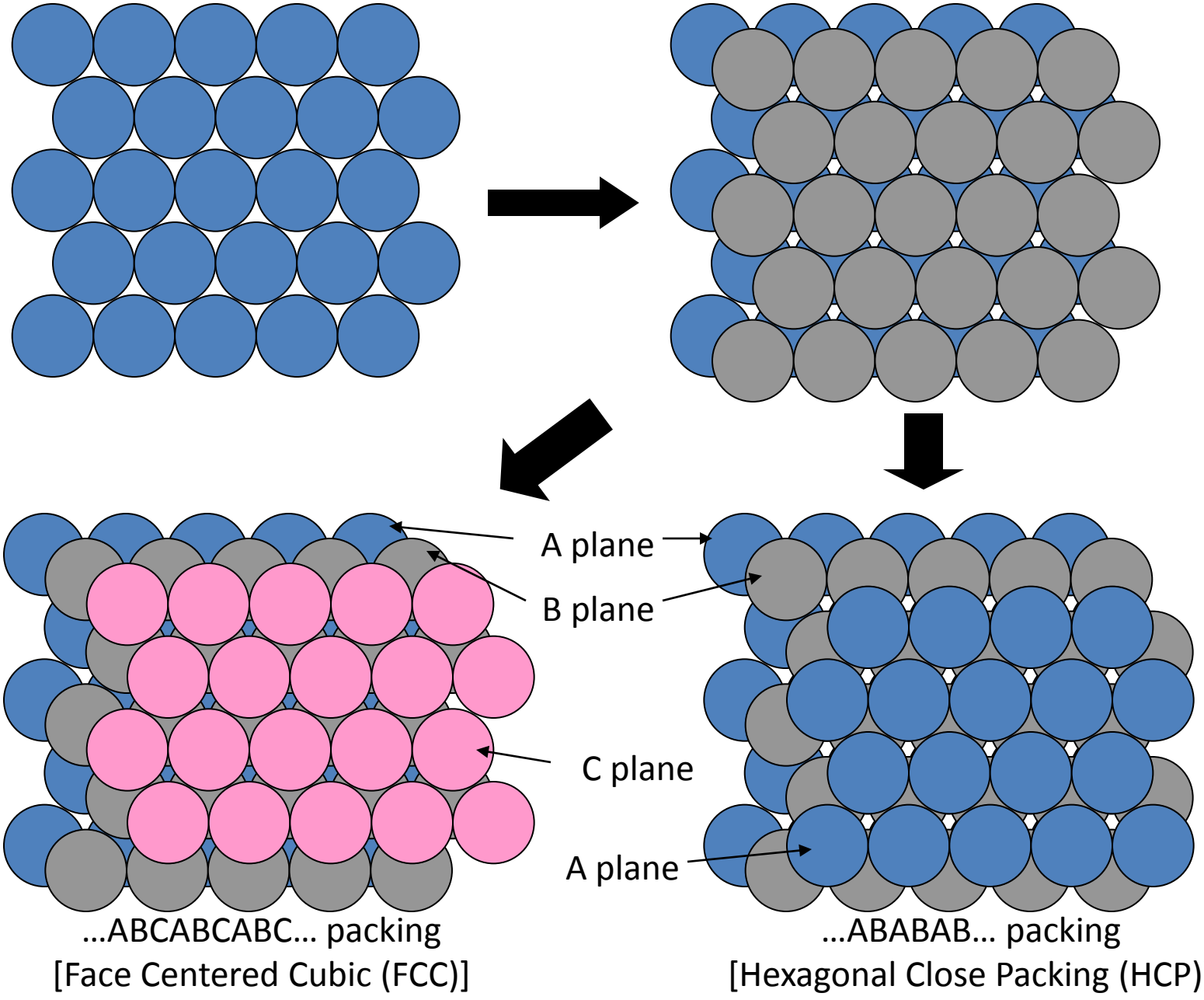
$$APF = \frac{\text{atoms}}{\text{unit cell}} \cdot \frac{\text{volume}}{\text{atom}} \Big/ \frac{\text{volume}}{\text{unit cell}}$$

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

- APF for a body-centered cubic structure = $\pi/(3\sqrt{2}) = 0.74$

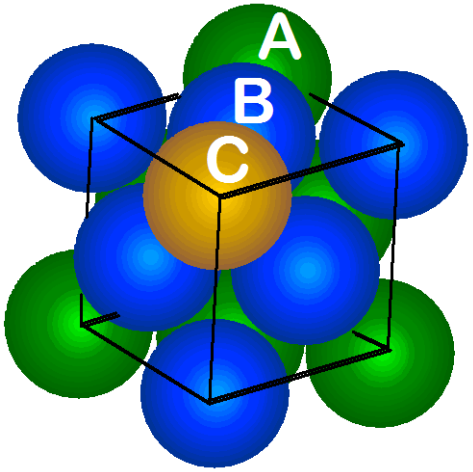
(best possible packing of identical spheres)

Close packed crystals

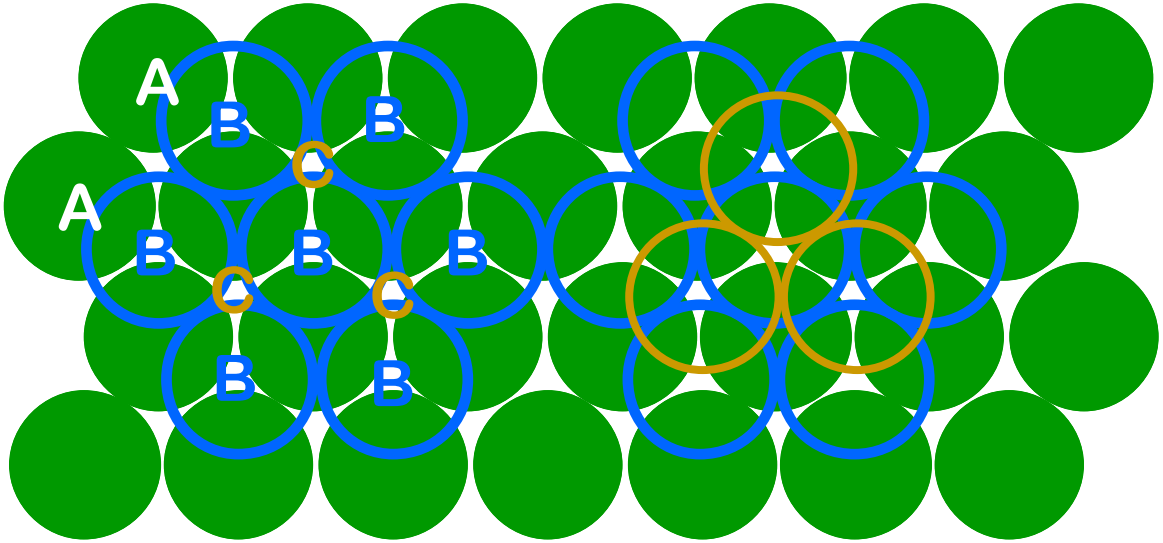


Close packing

FCC STACKING SEQUENCE



- FCC Unit Cell
- ABCABC... Stacking Sequence
- 2D Projection



HEXAGONAL CLOSE-PACKED STRUCTURE (HCP)

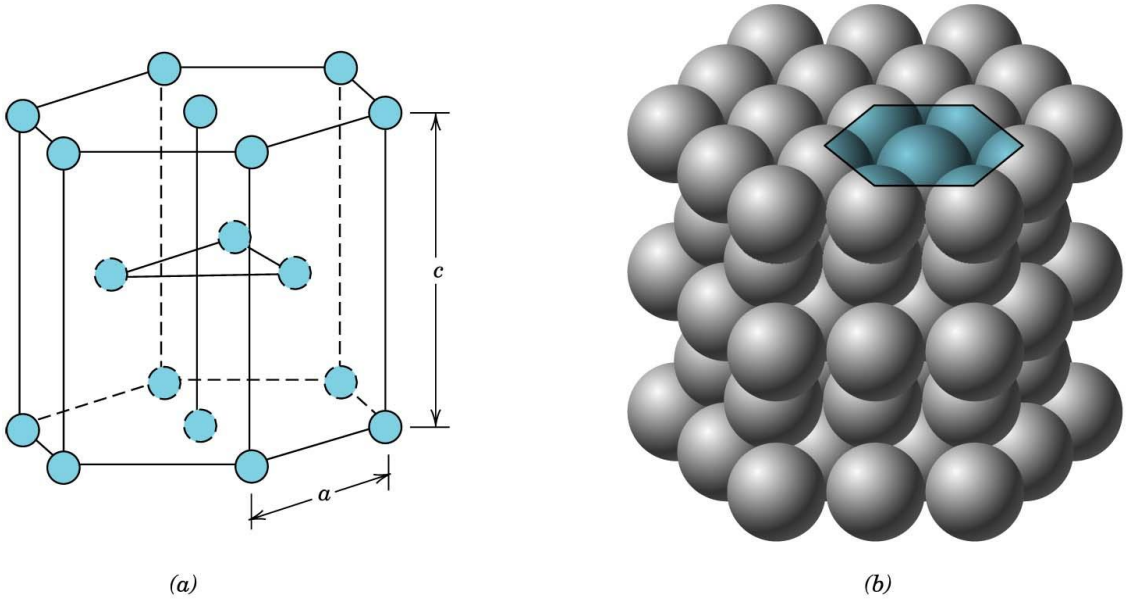


FIGURE 3.3 For the hexagonal close-packed crystal structure, (*a*) a reduced-sphere unit cell (*a* and *c* represent the short and long edge lengths, respectively), and (*b*) an aggregate of many atoms. (Figure *b* from W. G. Moffatt, G. W. Pearsall, and J. Wulff, *The Structure and Properties of Materials,* Vol. I, *Structure,* p. 51. Copyright © 1964 by John Wiley & Sons, New York. Reprinted by permission of John Wiley & Sons, Inc.)

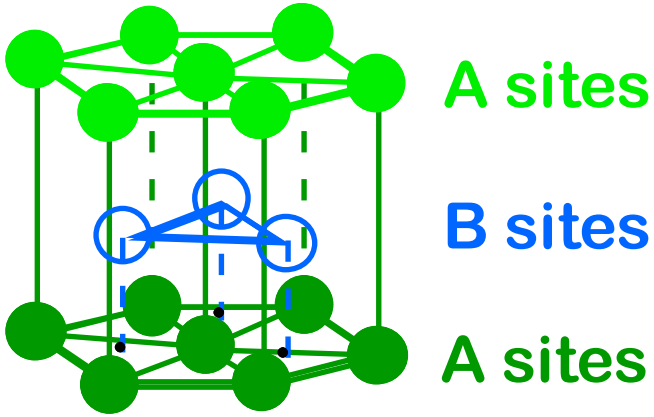
Ideally, c/a = 1.633 for close packing

However, in most metals, c/a ratio deviates from this value

HEXAGONAL CLOSE-PACKED STRUCTURE (HCP)

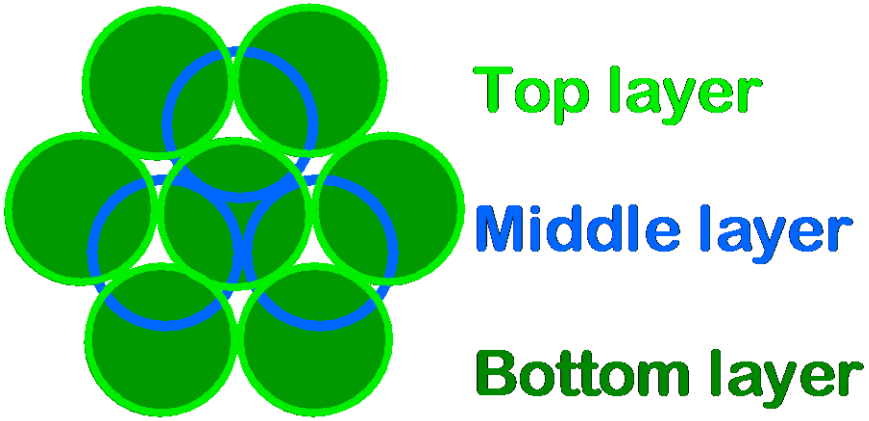
- ABAB... Stacking Sequence

- 3D Projection



Adapted from Fig. 3.3, *Callister 6e.*

- 2D Projection

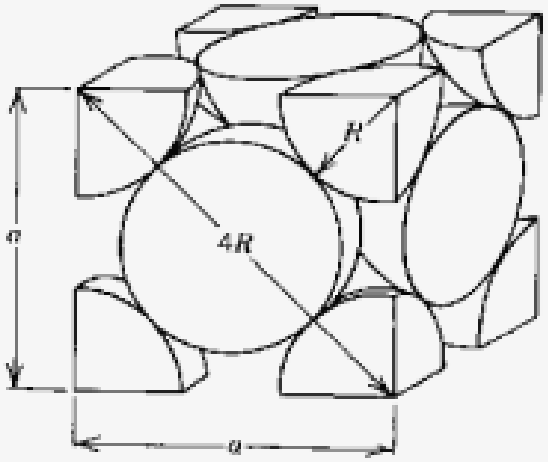


- Coordination # = 12

- APF = 0.74, for ideal c/a ratio of 1.633

Example: Calculate the volume of an FCC unit cell in terms of the atomic radius R.

Solution. In the FCC unit cell illustrated,



the atoms touch one another across a face diagonal, the length of which is $4R$. Since the unit cell is a cube, its volume is a^3, where a is the cell edge length. From the right triangle on the face

$$a^2 + a^2 = (4R)^2$$

or, solving for a,

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

The FCC unit cell volume V_C may be computed from

$$V_C = a^3 = (2R\sqrt{2})^3 = 16R^3\sqrt{2}$$

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Example: Show that the atomic packing factor for the FCC crystal structure is 0.74

Solution. The APF is defined as the fraction of solid sphere volume in a unit cell, or

$$\text{APF} = \frac{\text{total sphere volume}}{\text{total unit cell volume}} = \frac{V_S}{V_C}$$

Both the total sphere and unit cell volumes may be calculated in terms of the atomic radius R. The volume for a sphere is $\frac{4}{3}\pi R^3$, and since there are four atoms per FCC unit cell, the total FCC sphere volume is

$$V_S = 4\,\frac{4}{3}\,\pi R^3 = \frac{16}{3}\,\pi R^3$$

From Example Problem 3.1, the total unit cell volume is

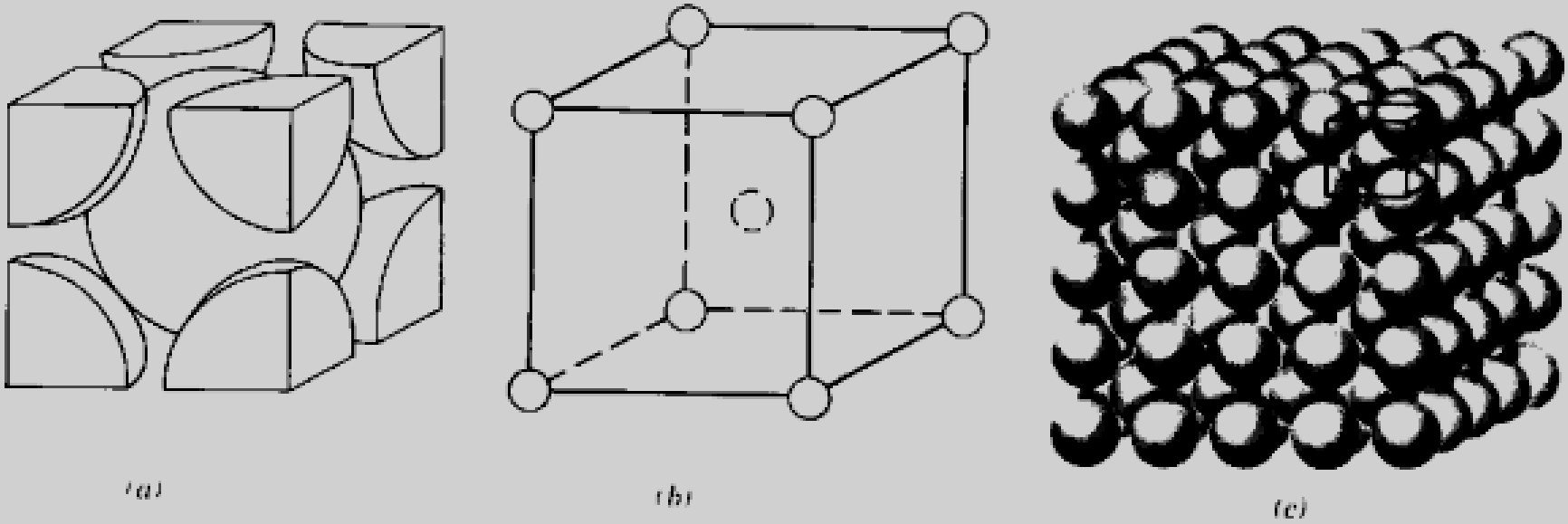
$$V_C = 16R^3\sqrt{2}$$

Therefore, the atomic packing factor is

$$\text{APF} = \frac{V_S}{V_C} = \frac{(16/3)\pi R^3}{16R^3\sqrt{2}} = 0.74$$

Body centered cubic structure

(chromium, iron, tungsten)
Packing Factor: 0.68 (volume of atoms in cell/total volume of cell)
2 atoms per unit cell
Coordination number 8 (# of adjacent atoms)



(a) (b) (c)

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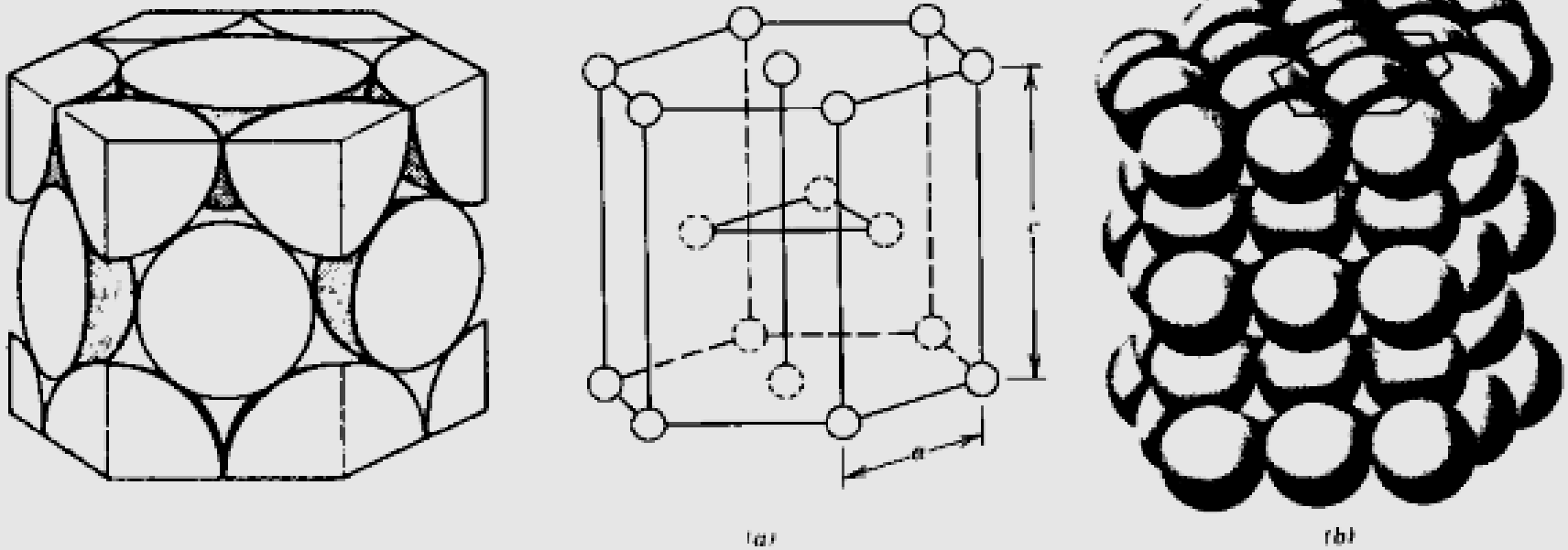
Hexagonal close packed structure

(cadmium, magnesium, titanium, zinc)
Packing Factor: 0.74 (volume of atoms in cell/total volume of cell)
6 atoms per unit cell
Coordination number 12 (# of adjacent atoms)



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COMPARISON OF CRYSTAL STRUCTURES

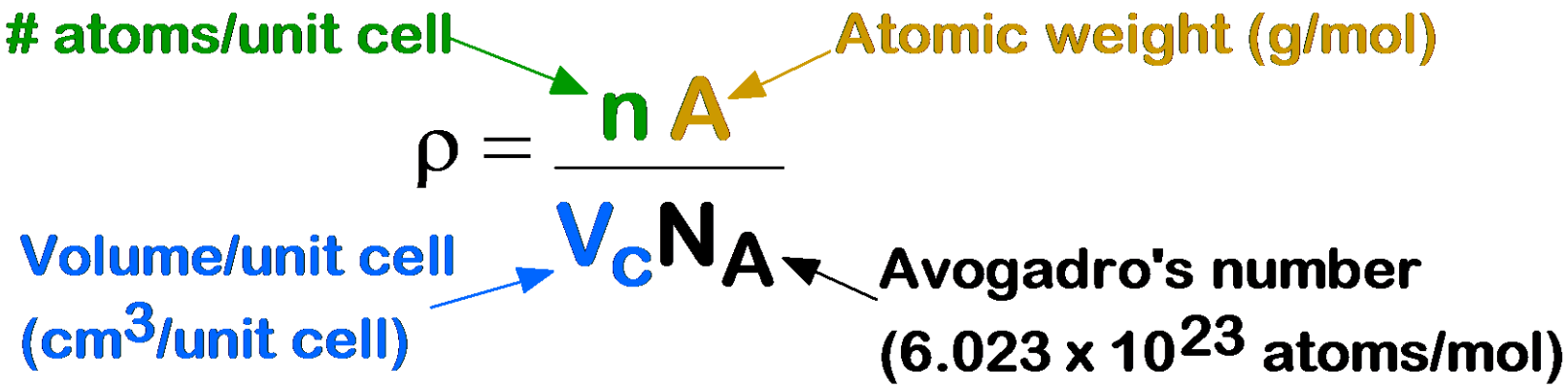
close packed directions	packing factor	coordination #	Crystal structure
cube edges	0.52	6	• Simple Cubic (SC)
body diagonal	0.68	8	• Body Centered Cubic (BCC)
face diagonal	0.74	12	• Face Centered Cubic (FCC)
hexagonal side	0.74	12	• Hexagonal Close Pack (HCP)

THEORETICAL DENSITY, ρ

Density = mass/volume

mass = number of atoms per unit cell * mass of each atom

mass of each atom = atomic weight/avogadro's number

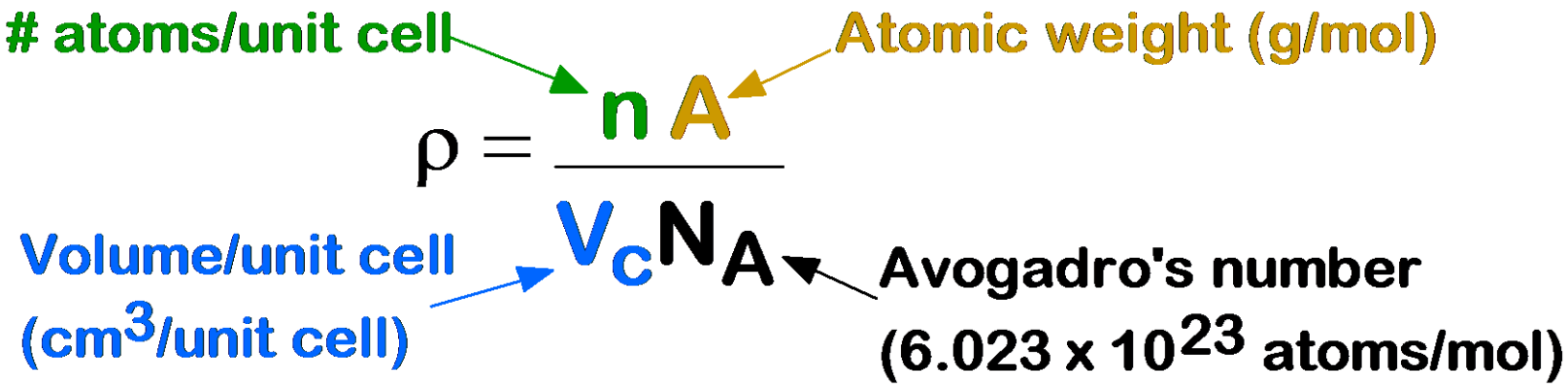


Characteristics of Selected Elements at 20C

Element	Symbol	At. Weight (amu)	Density (g/cm^3)	Crystal Structure	Atomic radius (nm)
Aluminum	Al	26.98	2.71	FCC	0.143
Argon	Ar	39.95	------	------	------
Barium	Ba	137.33	3.5	BCC	0.217
Beryllium	Be	9.012	1.85	HCP	0.114
Boron	B	10.81	2.34	Rhomb	------
Bromine	Br	79.90	------	------	------
Cadmium	Cd	112.41	8.65	HCP	0.149
Calcium	Ca	40.08	1.55	FCC	0.197
Carbon	C	12.011	2.25	Hex	0.071
Cesium	Cs	132.91	1.87	BCC	0.265
Chlorine	Cl	35.45	------	------	------
Chromium	Cr	52.00	7.19	BCC	0.125
Cobalt	Co	58.93	8.9	HCP	0.125
Copper	Cu	63.55	8.94	FCC	0.128
Flourine	F	19.00	------	------	------
Gallium	Ga	69.72	5.90	Ortho.	0.122
Germanium	Ge	72.59	5.32	Dia. cubic	0.122
Gold	Au	196.97	19.32	FCC	0.144
Helium	He	4.003	------	------	------
Hydrogen	H	1.008	------	------	------

Adapted from Table, "Characteristics of Selected Elements", inside front cover, *Callister 6e.*

THEORETICAL DENSITY, ρ



Example: Copper

Data from Table inside front cover of Callister (see previous slide):

- crystal structure = FCC: 4 atoms/unit cell
- atomic weight = 63.55 g/mol (1 amu = 1 g/mol)
- atomic radius R = 0.128 nm (1 nm = 10^{-7} cm)

$V_C = a^3$; For FCC, $a = 4R/\sqrt{2}$; $V_C = 4.75 \times 10^{-23} cm^3$

Result: theoretical $\rho_{Cu} = 8.89$ g/cm^3

Compare to actual: $\rho_{Cu} = 8.94$ g/cm^3