Chapter 3

The Structure of Crystalline Solids Part A

The University of Jordan
Chemical Engineering Department
First Semester 2022
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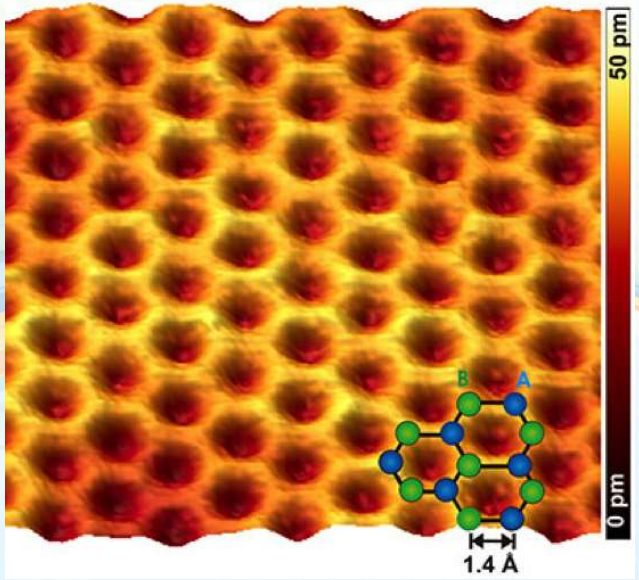
LOW POLY
BRAIN
box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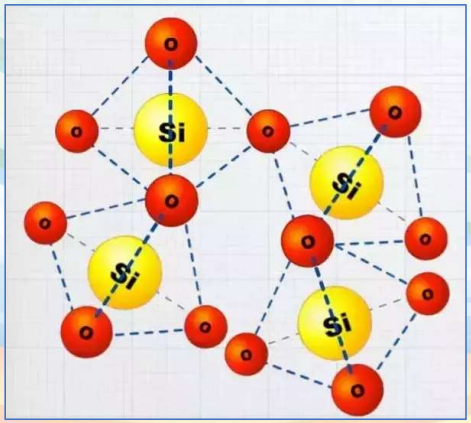
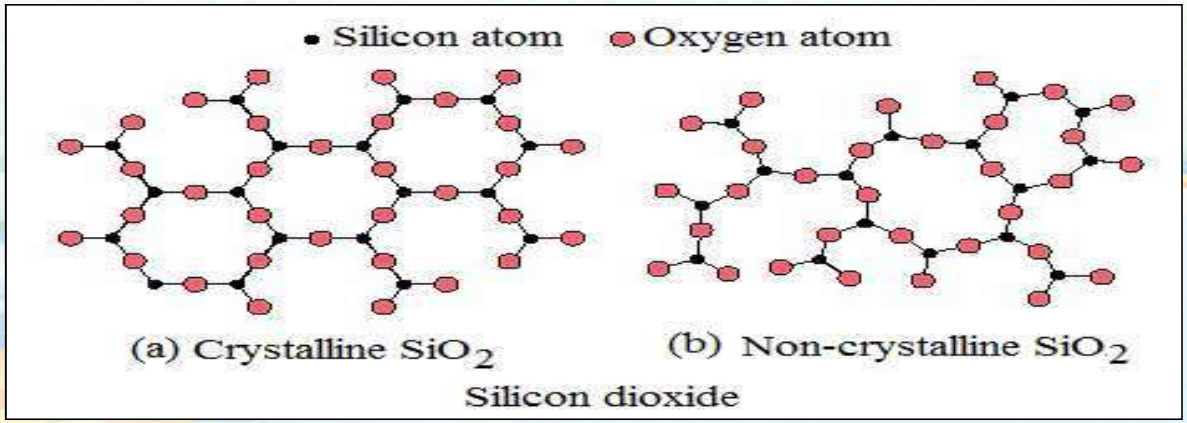
Outline

- How do atoms arrange themselves to form solids?
- Types of solids
  1. Single crystal
  2. Polycrystalline
  3. Amorphous
- Fundamental concepts
- Unit cells
- Crystal structures
  1. Simple cubic
  2. Face-centered cubic
  3. Body-centered cubic
  4. Hexagonal close-packed
- Close packed crystal structures
- Density computations

Types of solids

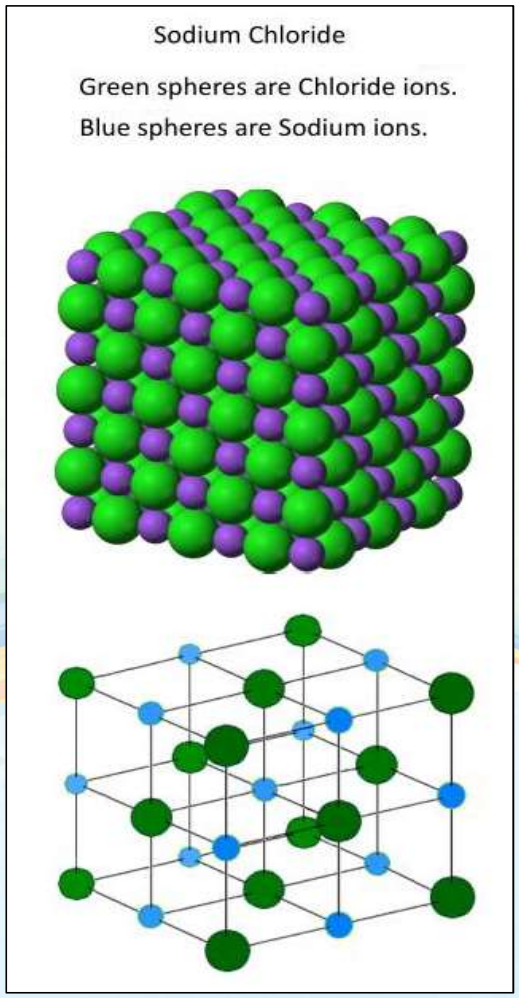
- *Crystalline material:* atoms self-organize in a periodic array:
  1. Single crystal: atoms are in a repeating or periodic array over the entire extent of the material
  2. Polycrystalline material: comprised of many small crystals or grains
- *Amorphous:* lacks a systematic atomic arrangement





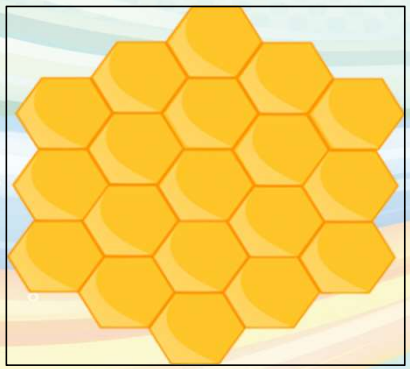
Crystal Structure

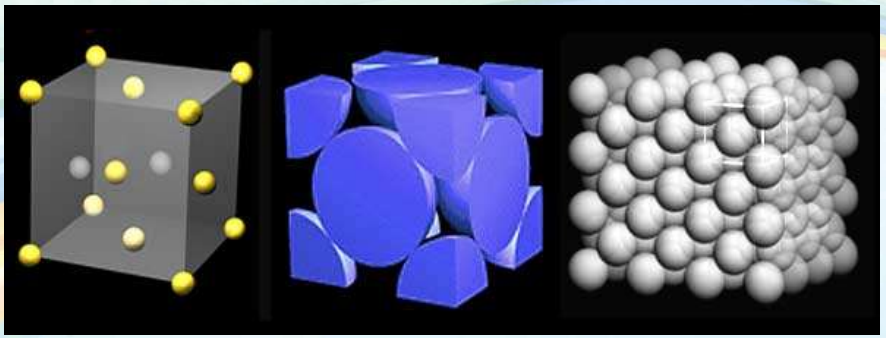
- To discuss crystalline structures it is useful to consider atoms as being hard spheres with well-defined radii.
- In this hard-sphere model, the shortest distance between two like atoms is one diameter.
- We can also consider crystalline structure as a lattice of points at atom/sphere centers.



Unit Cell

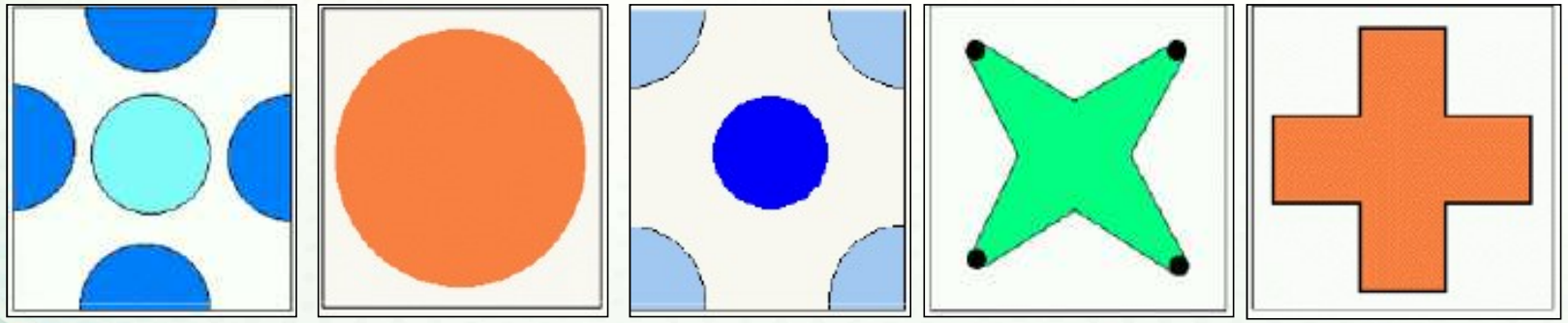
- The unit cell is the smallest structural unit or building block that can describe the crystal structure.
- Repetition of the unit cell generates the entire crystal.
- Example: 2D honeycomb net can be represented by translation of two adjacent atoms that form a unit cell for this 2D crystalline structure.



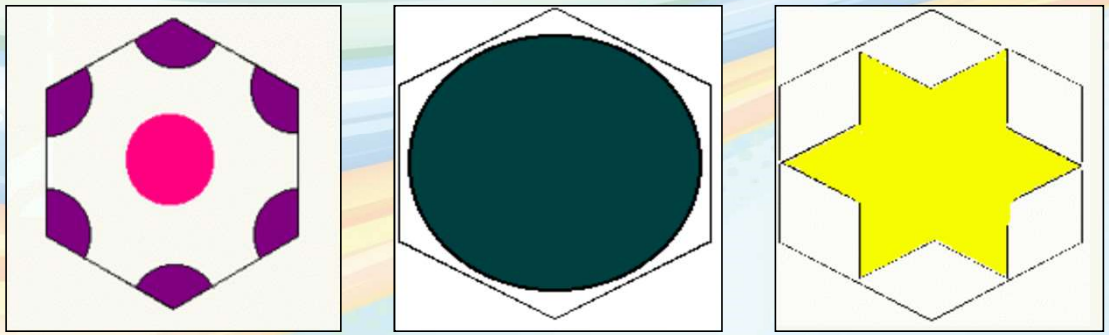


Example of 3D crystalline structure:

- *Different choices of unit cells are possible, for example:*
  A square unit cell may contain any of the following object patterns.



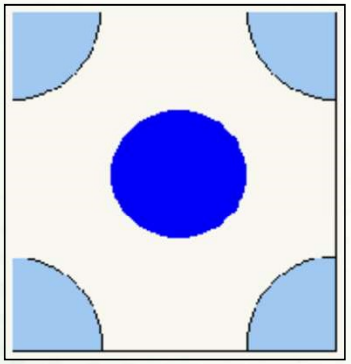
- *One hexagonal unit cell might look like any of the following.*



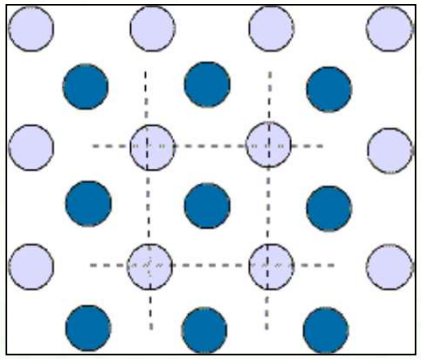
Crystalline Lattices

- A crystal is a repeating array. In describing this structure we must distinguish between the pattern of repetition (the lattice type) and what is repeated (the unit cell).
- The most fundamental property of a crystal lattice is its symmetry. If we initially limit ourselves to 2 dimensions for simplicity, three types are present:

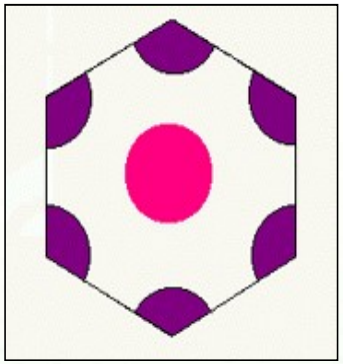
1. Squares
2. Rectangles
3. Hexagons



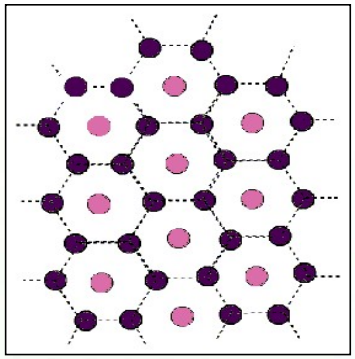
unit cell



lattice



unit cell



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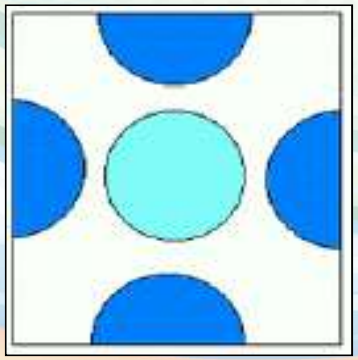
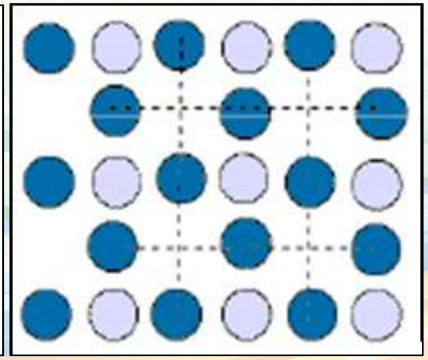


unit cell



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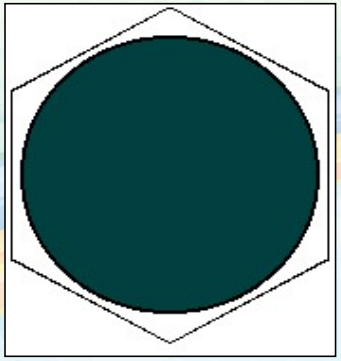
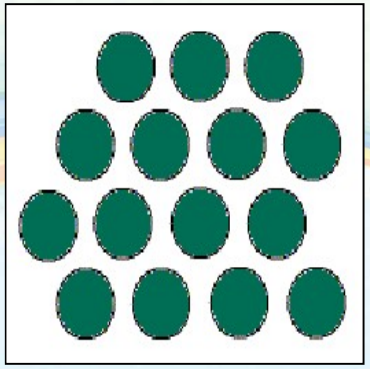


unit cell



lattice

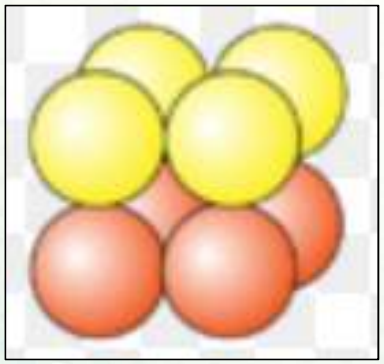
Metallic Crystal Structures

- Metals tend to be densely packed.
- Reasons for dense packing:
  - Typically, only one element is present, so all atomic radii are the same.
- Metals tend to be densely packed.
  - Metallic bonding is not directional.
  - Nearest neighbor distances tend to be small in order to lower bond energy.
- Have the simplest crystal structures.

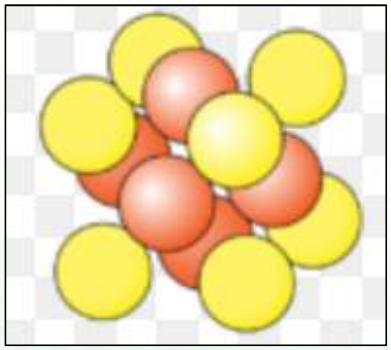
- *Metals are usually (poly)crystalline.*
- *Although formation of amorphous metals is possible by rapid cooling.*
- *The atomic bonding in metals is non-directional ⇒ no restriction on numbers or positions of nearest-neighbor atoms ⇒ large number of nearest neighbors and dense atomic packing.*
- *Atom (hard sphere) radius, R, defined by ion core radius - typically 0.1 - 0.2 nm*

The most common types of unit cells are:

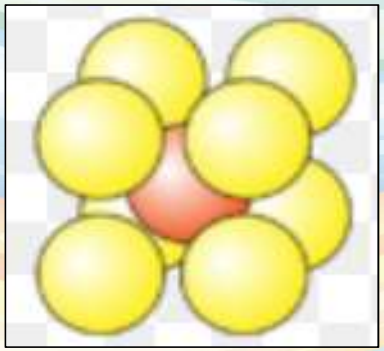
1- The simple cubic (SC)



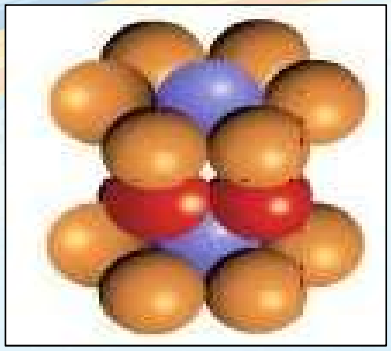
2- The faced centered cubic (FCC).



3- The body-centered cubic (BCC)



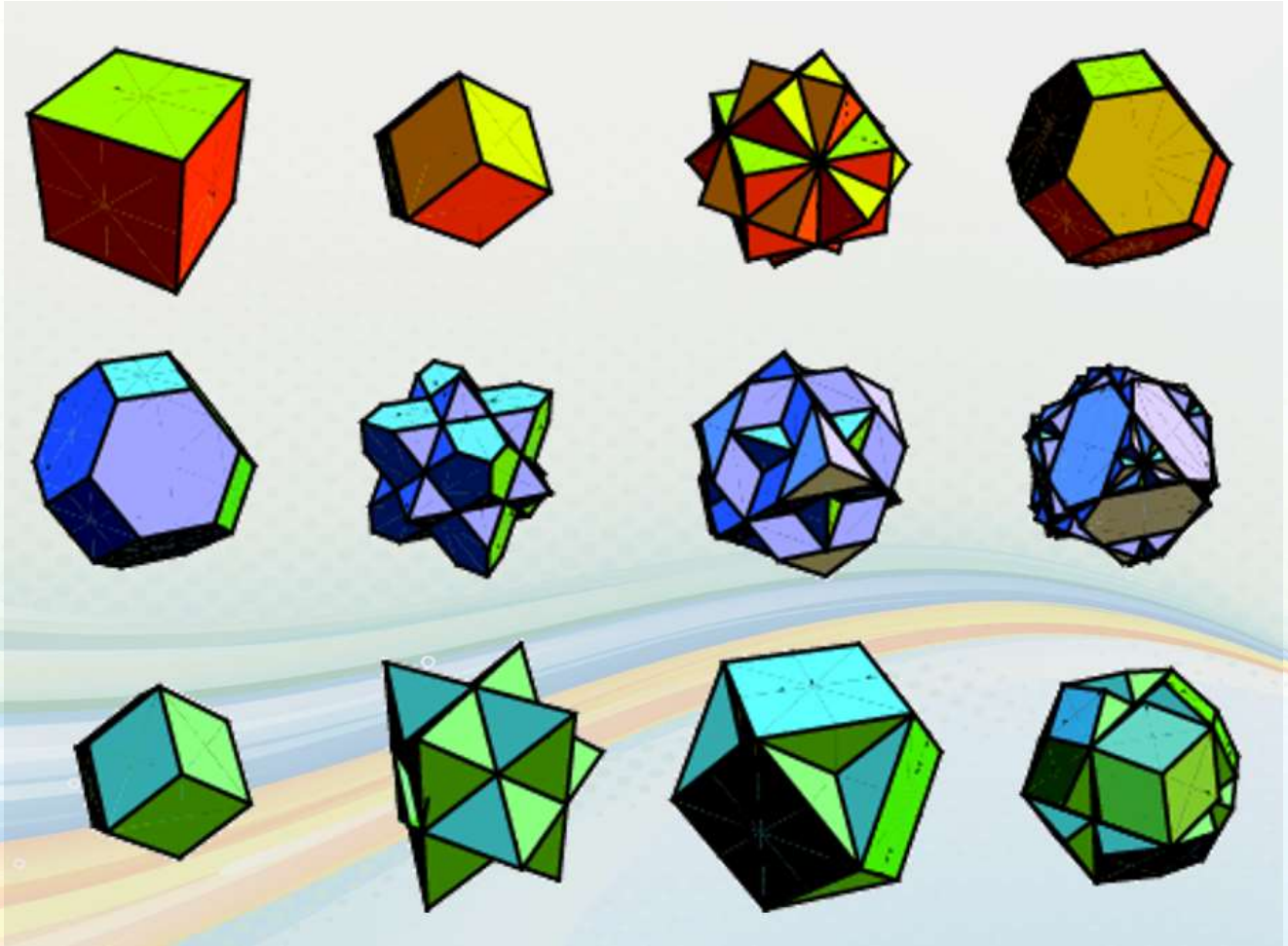
4- The hexagonal close-packed (HCP)



Simple cubic

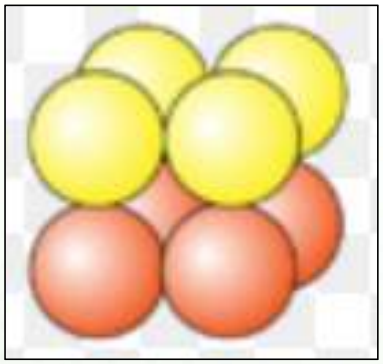
Faced centered cubic

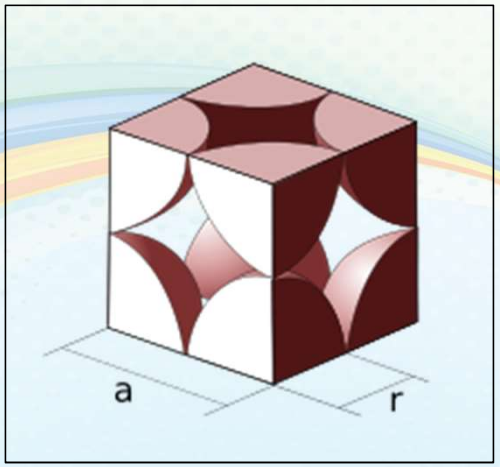
Body-centered cubic

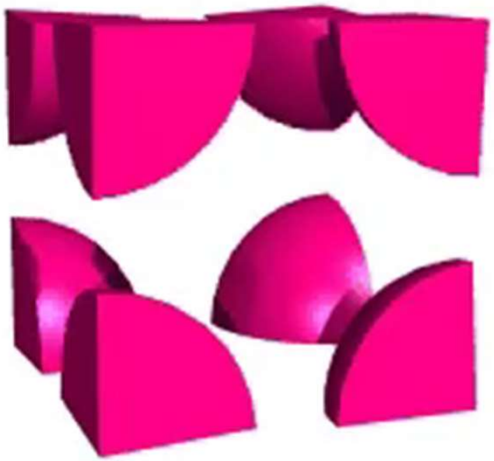


Simple Cubic Metal

- Rare due to low packing density.
  - Only Po has this structure.
  - Close-packed directions are cube edges.
- In a metal the atoms are all identical, and most are spherical (the bonding does not depend on direction).
- Metals thus tend to adopt relatively simple structures. The simplest is simple cubic.



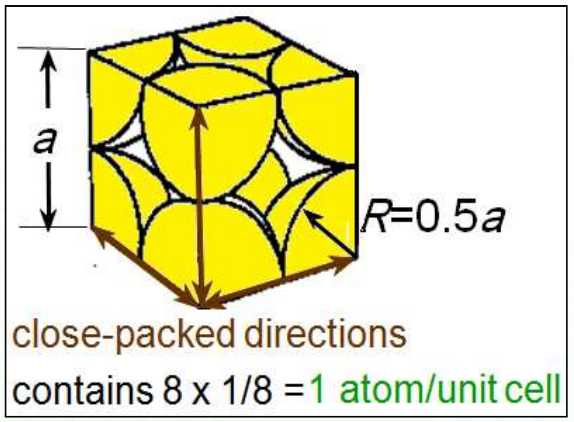




- Coordination number = 6 atoms
- Number of atoms per unit cell:

  = 8 corners x 1/8

  = 1 atoms

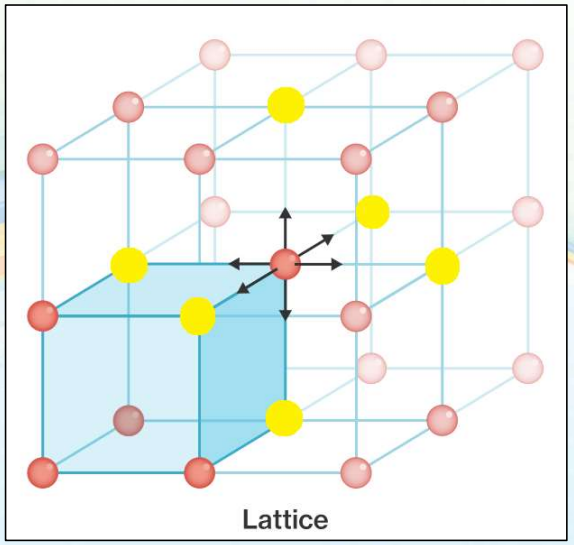


- In 3-D the packing efficiency is given by :
  - ✓ P.E. = (Volume of spheres) / (volume of cell)
  - ✓ For a simple cubic lattice, this is:

$$Volume\ of\ spheres = \frac{1}{8} \times 8 \times \frac{4}{3} \times \frac{22}{7} \times (0.5a)^3$$

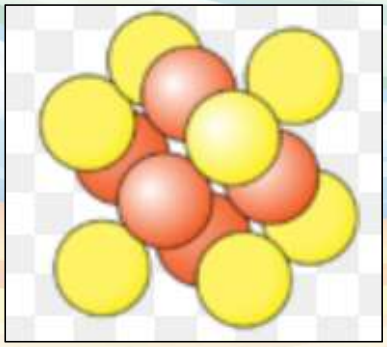
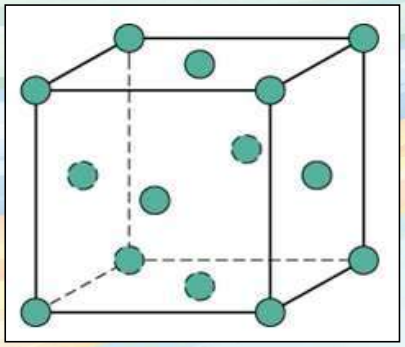
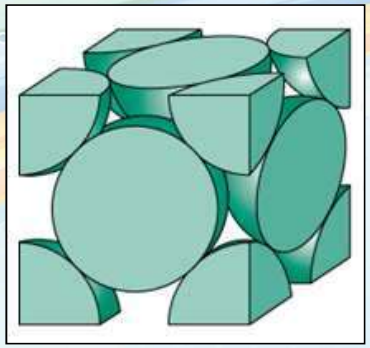
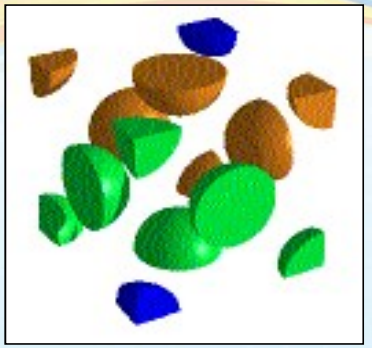
$$Volume\ of\ cell = (a)^3$$

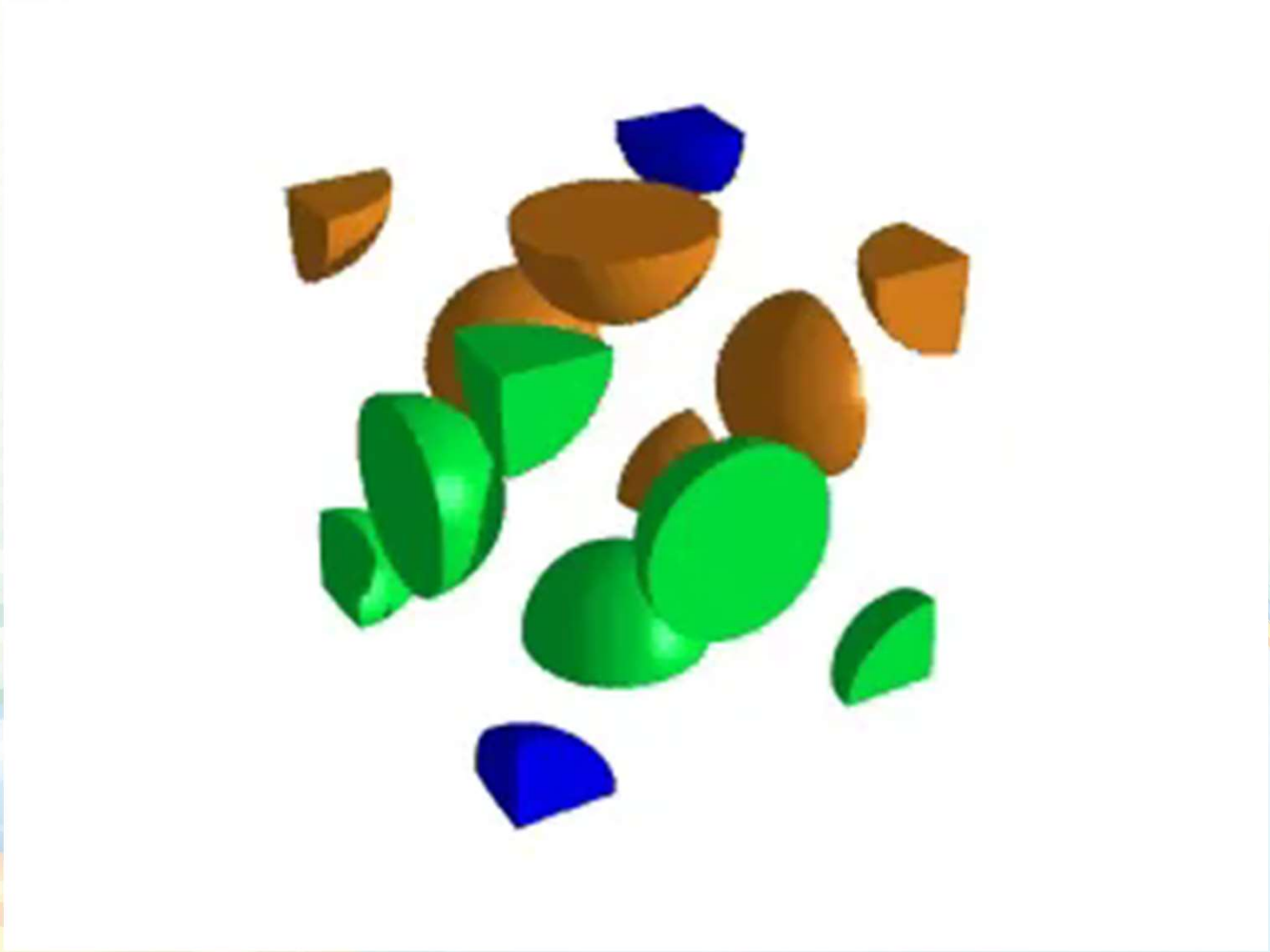
$$\therefore P.E. = \frac{88}{168} = 0.523$$

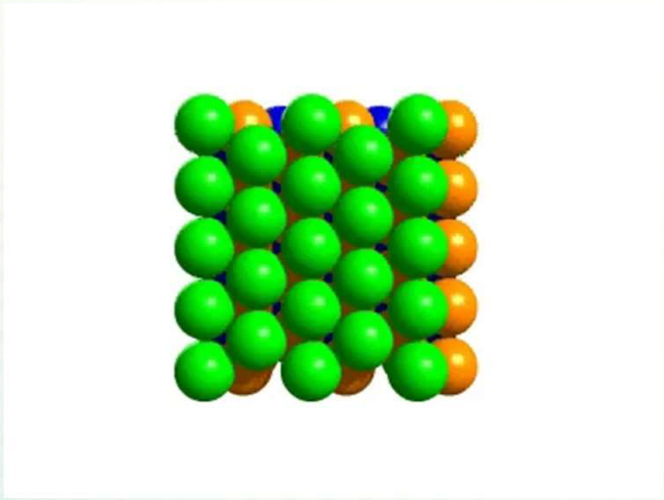


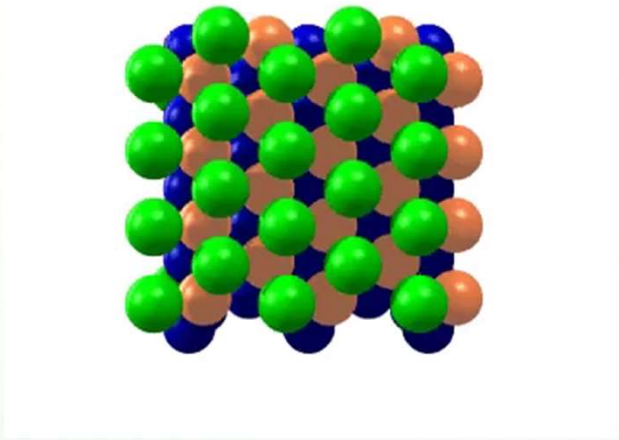
Face Centered Cubic (FCC)
or
Cubic Close Packed (CCP)

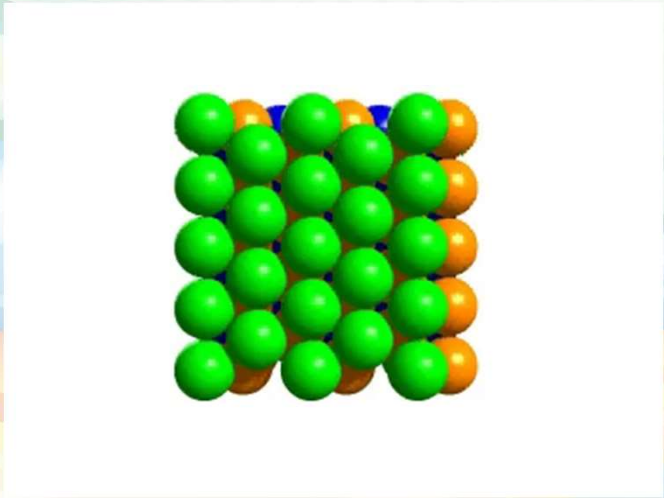
- Think of this cell as being made by inserting another atom into each face of the simple cubic lattice - hence the "face centered cubic" name .
- The reason for the various colors is to help point out how the cells stack in the solid .

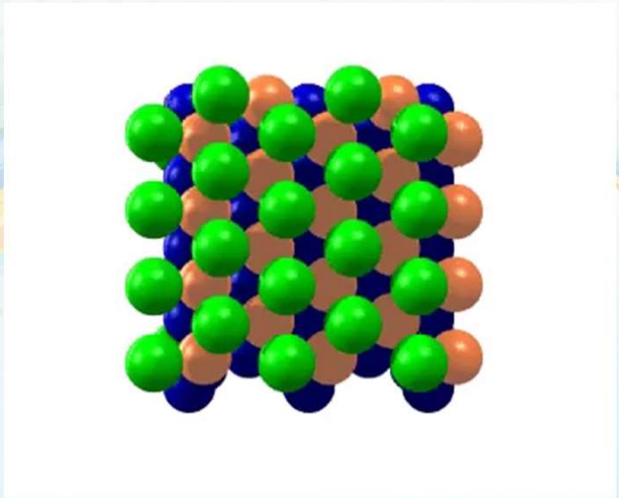









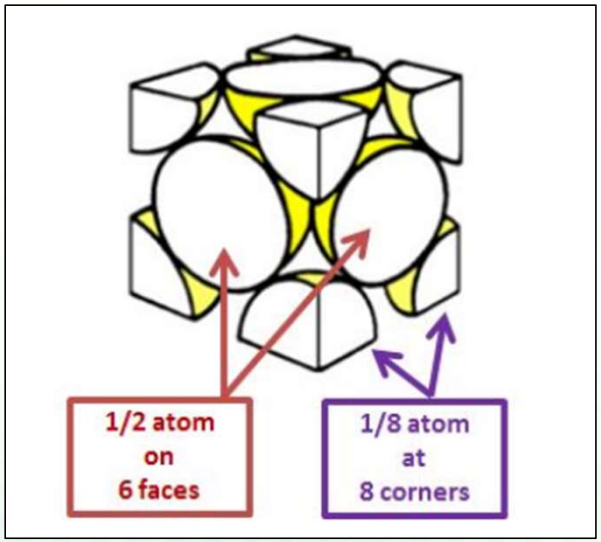


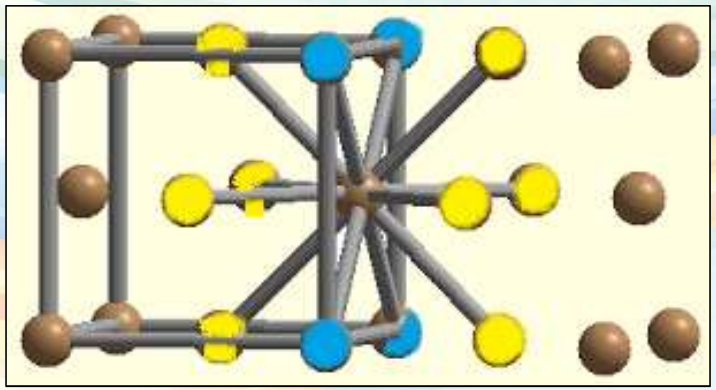


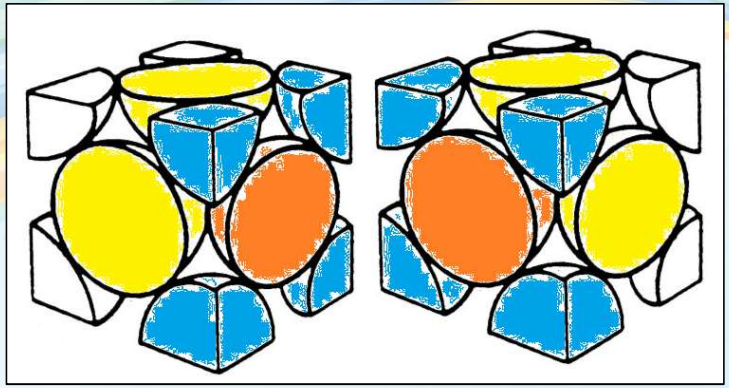


- *Atoms touch each other along face diagonals.*
  - ✓ *Note: All atoms are identical.*
- *Example:*
  - ✓ *Al, Cu, Au, Pb, Ni, Pt, Ag*
- *Coordination number = 12 atoms*
- *Number of atoms per unit cell:*

  = 6 face x 1/2 + 8 corners x 1/8 = 4





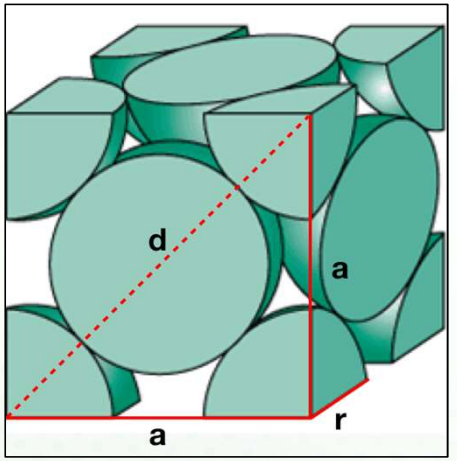


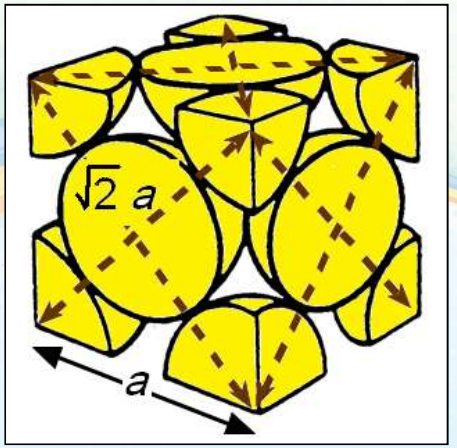
- *In 3-D the packing efficiency is given by :*
  - ✓ *P.E. = (Volume of spheres) / (volume of cell)*
- *For a face centered cubic lattice, this is:*

$$Volume\ of\ spheres = 4 \times \frac{4}{3} \times \frac{22}{7} \times \left(\frac{a\sqrt{2}}{4}\right)^3$$

$$Volume\ of\ cell = (a)^3$$

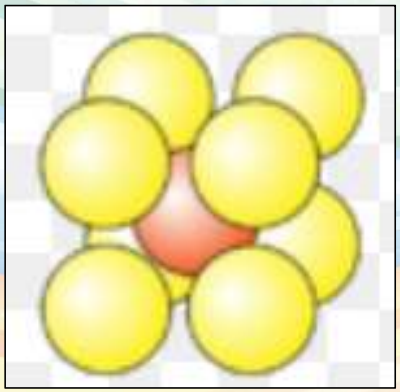
$$\therefore P.E. = \frac{995.6}{1344} = 0.7405$$

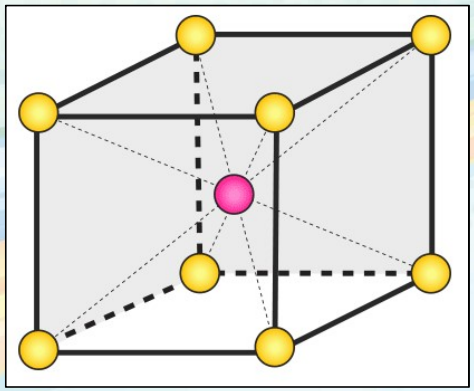


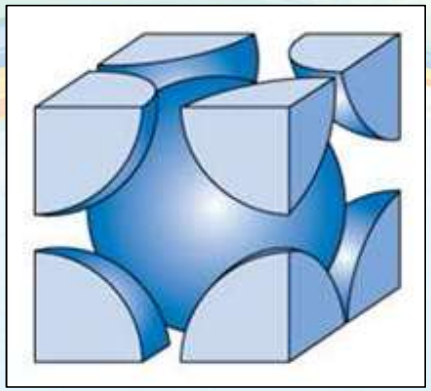


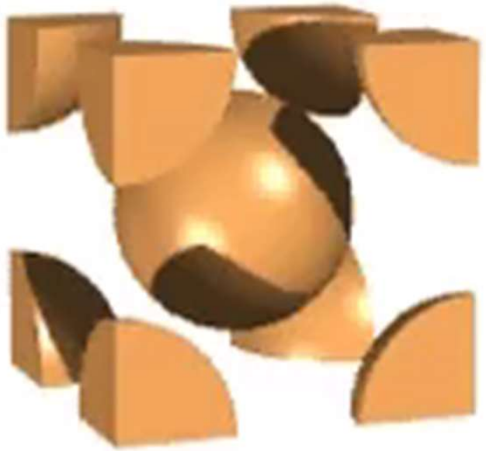
Body Centered Cubic Structure (BCC)

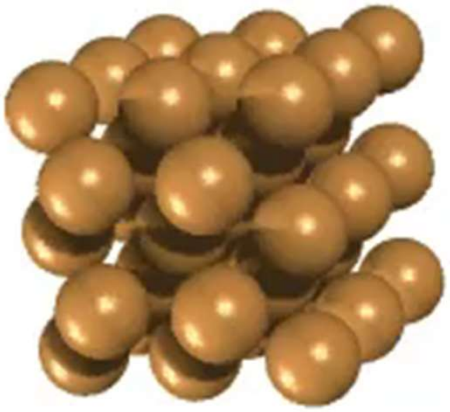
- Think of this unit cell as made by stuffing another atom into the center of the simple cubic lattice, slightly spreading the corners.
- The corner spheres no longer quite touch one another, but do touch the center.
- Examples: Cr, W, Fe (α), Tantalum, Molybdenum







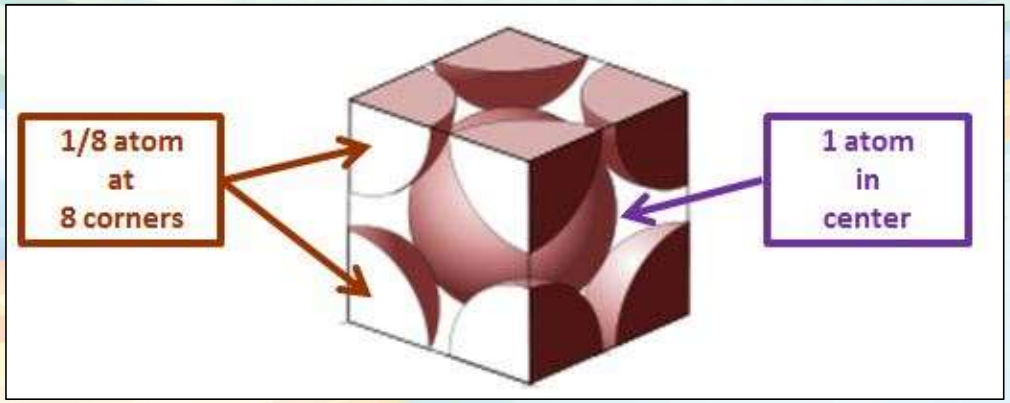


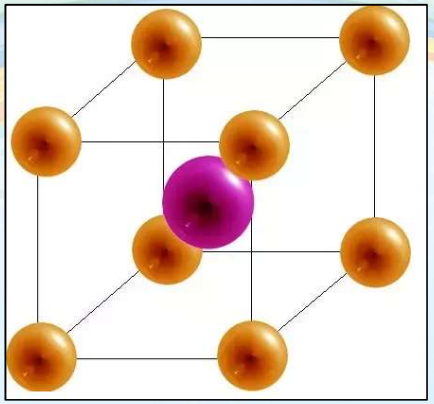


- *The hard spheres touch one another along cube diagonal*
- *The coordination number, CN = 8*
- *Number of atoms per unit cell, n = 2*

  1 center atom shared by no other cells: 1 x 1 = 1

  8 corner atoms shared by eight cells: 8 x 1/8 = 1
- *Corner and center atoms are equivalent*





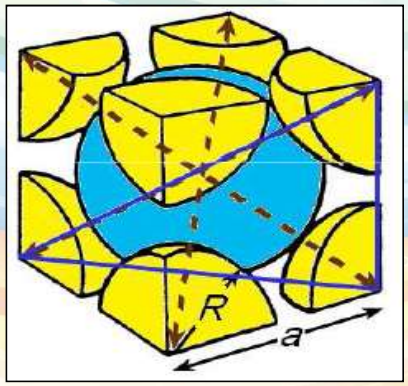
⇒ *the cube edge length, a= 4R/√3*

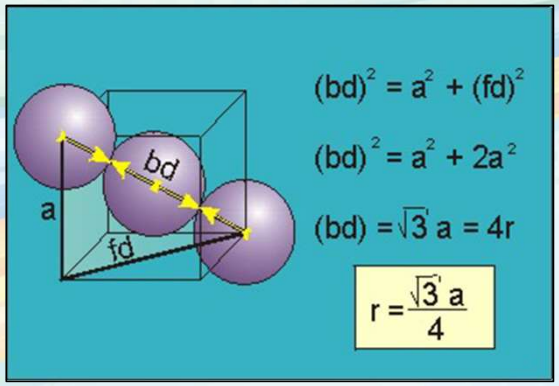
$$Volume\ of\ spheres = 2 \times \frac{4}{3} \times \frac{22}{7} \times \left(\frac{a\sqrt{3}}{4}\right)^3$$

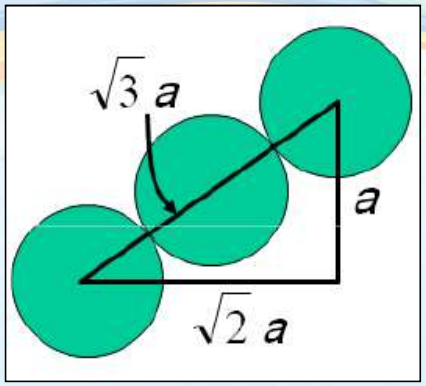
$$Volume\ of\ cell = (a)^3$$

$$\therefore P.E. = \frac{914.5}{1344} = 0.6805$$

- *The higher coordination number and packing efficiency mean that this lattice uses space more efficiently than simple cubic.*

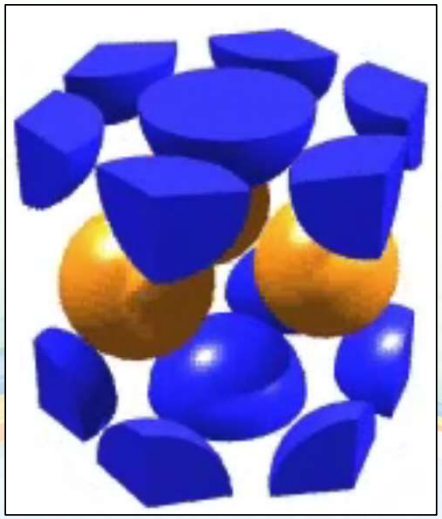


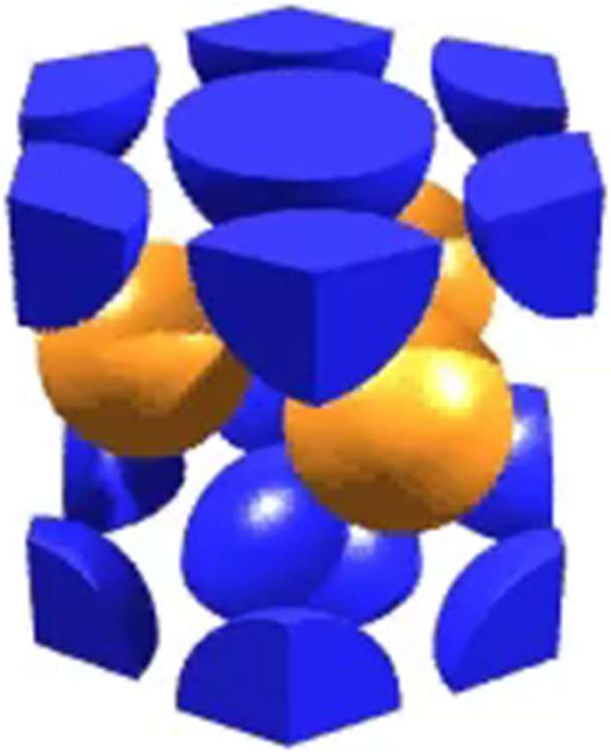




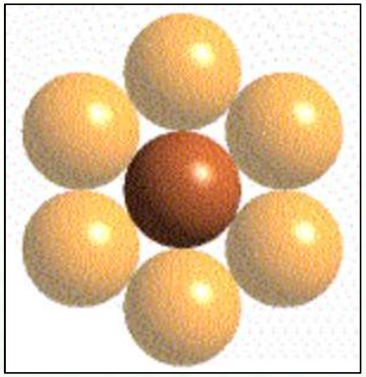
Hexagonal Close- Packed Crystal Structure

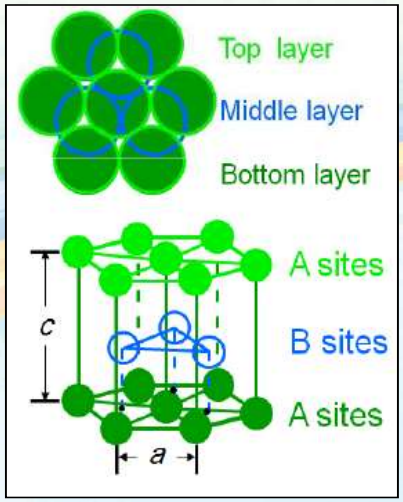
- HCP is one more common structure of metallic crystals.
- Six atoms form regular hexagon, surrounding one atom in center.
- Another plane is situated halfway up unit cell (c-axis), with 3 additional atoms situated at interstices of hexagonal (close-packed) planes.
- Example: Cd, Mg, Zn, Ti have this crystal structure.

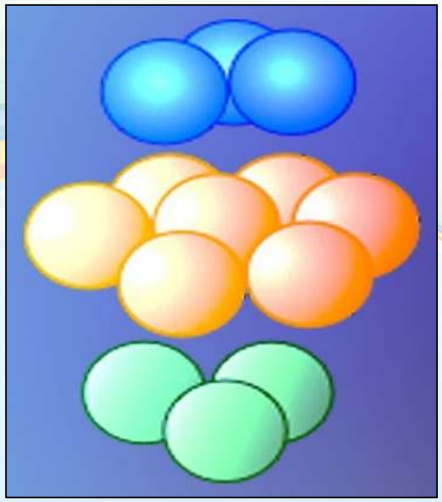




- The hexagonal close packed structure can be made by piling layers in the A - B - A - B - A - B . . . . . sequence.
- Unit cell has two lattice parameters a and c.
- Ratio c/a = 1.633
- The coordination number, CN = 12
- Number of atoms per unit cell, n= 6.
  - ✓ 3 mid-plane atoms shared by no other cells: 3 x 1 = 3
  - ✓ 12 hexagonal corner atoms shared by 6 cells: 12 x 1/6 = 2
  - ✓ 2 top/bottom plane center atoms shared by 2 cells: 2 x 1/2 = 1







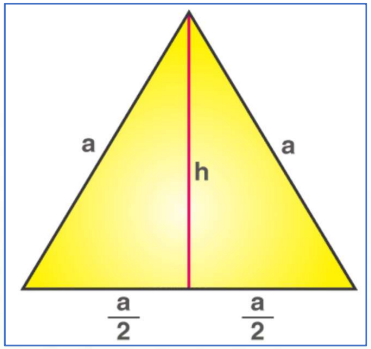
- *In 3-D the packing efficiency is given by :*
  - ✓ *P.E. = (Volume of spheres) / (volume of cell)*

$$Volume\ of\ spheres = 6 \times \frac{4}{3} \times \frac{22}{7} \times (r)^3$$

$$Volume\ of\ spheres = 25.1428(r)^3$$

$$Volume\ of\ cell = 24\sqrt{2}(r)^3$$

$$\therefore P.E. = 0.7405$$



$a^2 = h^2 + (a/2)^2$

$\Rightarrow h^2 = a^2 - a^2/4$

$\Rightarrow h^2 = (3a^2)/4$

Or, $h = ½(\sqrt{3}a)$

Area of Triangle = ½ × base × height

$\Rightarrow A = ½ \times a \times ½(\sqrt{3}a)$

Density Computations

- Since the entire crystal can be generated by the repetition of the unit cell, the density of a crystalline material,

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

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

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

Characteristics of Selected Elements

Element	*Symbol*	*Atomic Number*	*Atomic Weight (amu)*	*Density of Solid, 20°C (g/cm^3)*	*Crystal Structure, 20°C*	*Atomic Radius (nm)*	*Ionic Radius (nm)*	*Most Common Valence*	*Melting Point (°C)*
Aluminum	Al	13	26.98	2.71	FCC	0.143	0.053	3+	660.4
Argon	Ar	18	39.95	—	—	—	—	Inert	−189.2
Barium	Ba	56	137.33	3.5	BCC	0.217	0.136	2+	725
Beryllium	Be	4	9.012	1.85	HCP	0.114	0.035	2+	1278
Boron	B	5	10.81	2.34	Rhomb.	—	0.023	3+	2300
Bromine	Br	35	79.90	—	—	—	0.196	1−	−7.2
Cadmium	Cd	48	112.41	8.65	HCP	0.149	0.095	2+	321
Calcium	Ca	20	40.08	1.55	FCC	0.197	0.100	2+	839
Carbon	C	6	12.011	2.25	Hex.	0.071	~0.016	4+	(sublimes at 3367)
Cesium	Cs	55	132.91	1.87	BCC	0.265	0.170	1+	28.4
Chlorine	Cl	17	35.45	—	—	—	0.181	1−	−101
Chromium	Cr	24	52.00	7.19	BCC	0.125	0.063	3+	1875
Cobalt	Co	27	58.93	8.9	HCP	0.125	0.072	2+	1495
Copper	Cu	29	63.55	8.94	FCC	0.128	0.096	1+	1085
Fluorine	F	9	19.00	—	—	—	0.133	1−	−220
Gallium	Ga	31	69.72	5.90	Ortho.	0.122	0.062	3+	29.8
Germanium	Ge	32	72.64	5.32	Dia. cubic	0.122	0.053	4+	937
Gold	Au	79	196.97	19.32	FCC	0.144	0.137	1+	1064
Helium	He	2	4.003	—	—	—	—	Inert	−272 (at 26 atm)
Hydrogen	H	1	1.008	—	—	—	0.154	1+	−259
Iodine	I	53	126.91	4.93	Ortho.	0.136	0.220	1−	114

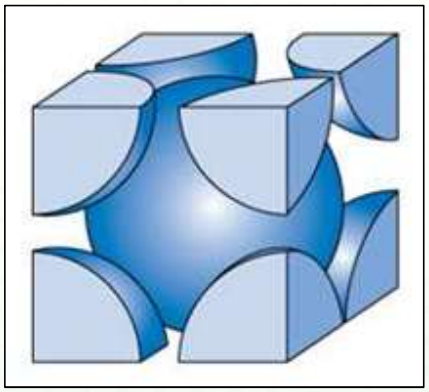
Theoretical Density, ρ

- Ex: Cr (BCC)

  $\mathcal{A}$ = 52.00 g/mol

  $\mathcal{R}$ = 0.125nm

  n = 2



$$a = \frac{4}{\sqrt{3}} R$$

$$a = \frac{4}{\sqrt{3}} (0.125) = 0.2887\ nm$$

$$\rho = \frac{2 \times 52.0}{(0.2887 \times 10^{-9})^3 \times 6.023 \times 10^{23}} = 7175961.9\ \frac{g}{m^3}$$

$$\rho = 7175961.9\ \frac{g}{m^3} \frac{m^3}{(100\ cm)^3} = 7.176\ \frac{g}{cm^3}$$ Theoretical

The actual density is 7.19

Densities of Materials Classes

In general:

$$\rho_{metals} > \rho_{ceramics} > \rho_{polymers}$$

Why?

Metals have:

- *Close-packed (metallic bonding)*
- *Often large atomic masses*

Ceramic have:

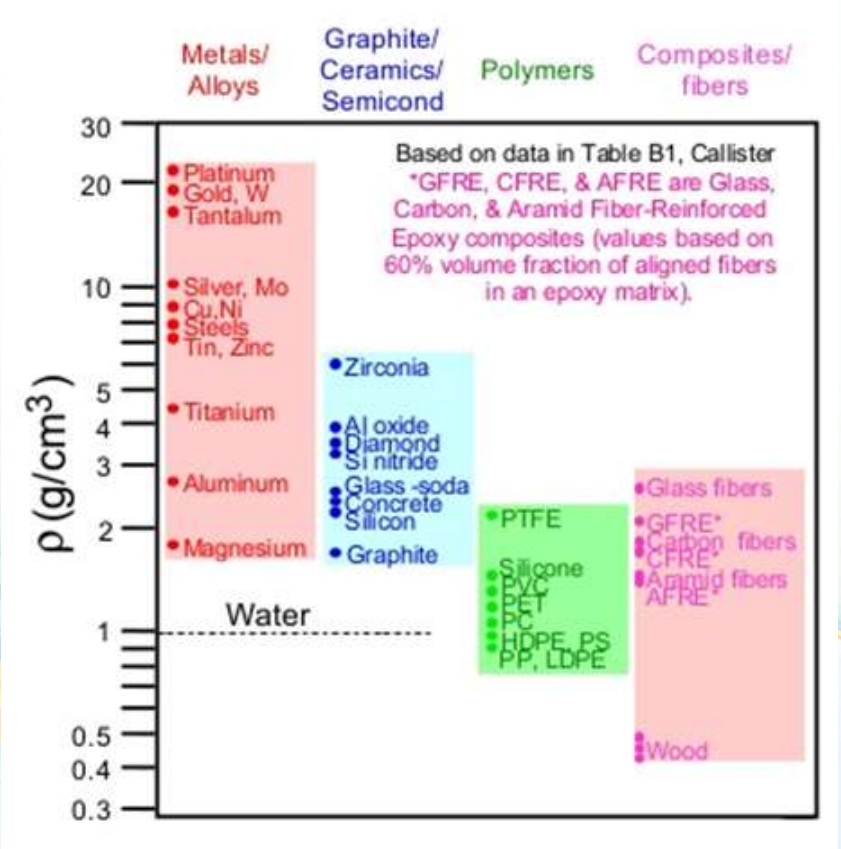
- *Less dense packing*
- *Often lighter elements*

Polymer have:

- *Low packing density (often amorphous)*
- *Lighter elements (C,H,O)*

Composites have:

- *Intermediate values*



Chapter 3

The Structure of Crystalline Solids Part B

The University of Jordan
Chemical Engineering Department
First Semester 2021
Prof. Yousef Mubarak

Outline

- Crystals as Building Blocks
- Isotropic OR Anisotropic
- Polymorphism and Allotropy
- Crystallographic Points, Directions, and Planes
  1. Symmetry Equivalent Directions
  2. POINT Coordinates
  3. Direction Coordinates
  4. How Do We Designate Lattice Planes?
- Linear Density
- Planar Density
- Designating Lattice Planes

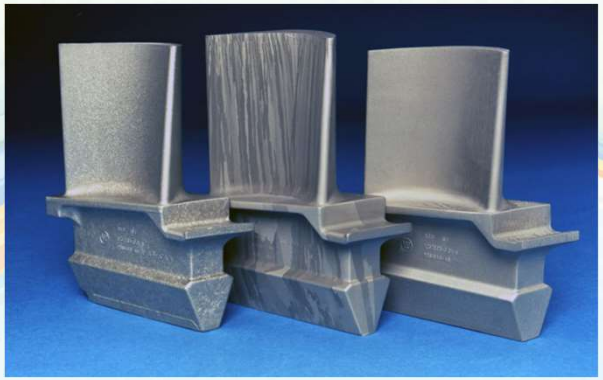
Crystals as Building Blocks

- Some engineering applications require single crystals:

Diamond single crystals for abrasives

- Properties of crystalline materials often related to crystal structure.

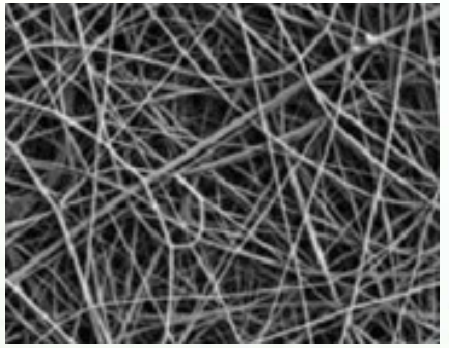
Ex: Quartz fractures more easily along some crystal planes than others.

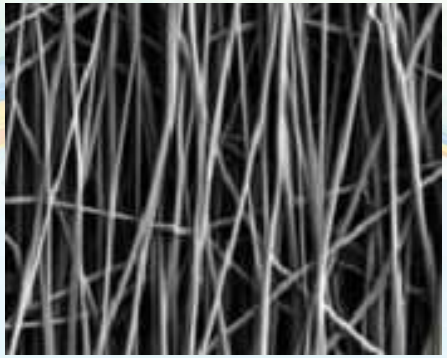


Turbine blades

Polycrystalline Materials

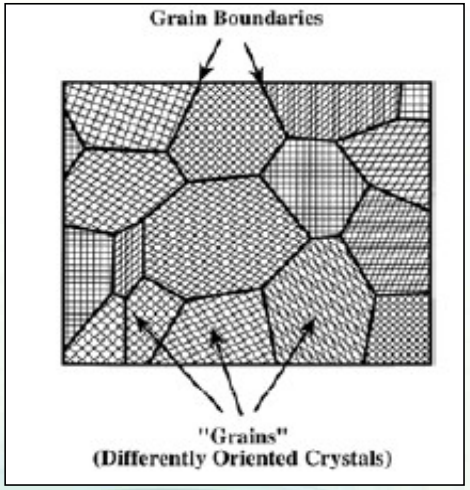
- Most engineering materials are polycrystalline.
- In polycrystalline materials, grain orientations are random, so bulk material properties are isotropic.
- Some polycrystalline materials have grains with preferred orientations (texture), so properties are dominated by those relevant to the texture orientation.
- If grains are randomly oriented, overall component properties are not directional.

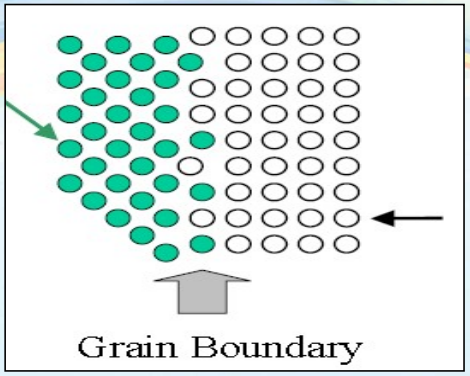




Single Crystals and Polycrystalline Materials

- *Single crystal:* atoms are in a repeating or periodic array over the entire extent of the material.
- *Polycrystalline material:* comprised of many small crystals or grains. The grains have different crystallographic orientation.
- There exist atomic mismatch within the regions where grains meet. These regions are called grain boundaries.



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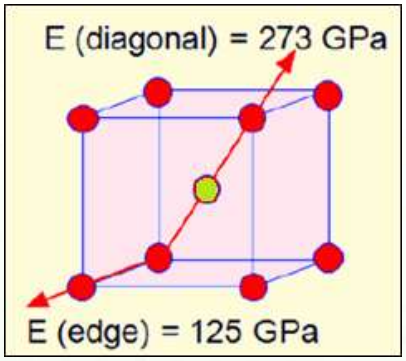
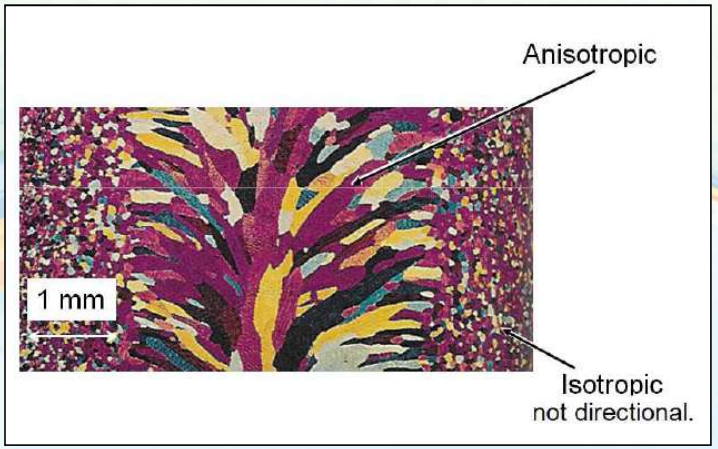
Single Crystals

- Properties vary with direction: anisotropic.
- Example: the modulus of elasticity E in BCC iron.



Polycrystals

- Properties may/may not vary with direction.
- If grains are randomly oriented: isotropic. ($E_{poly\ iron}$ = 210 GPa)
- If grains are textured, anisotropic.



Isotropic OR Anisotropic

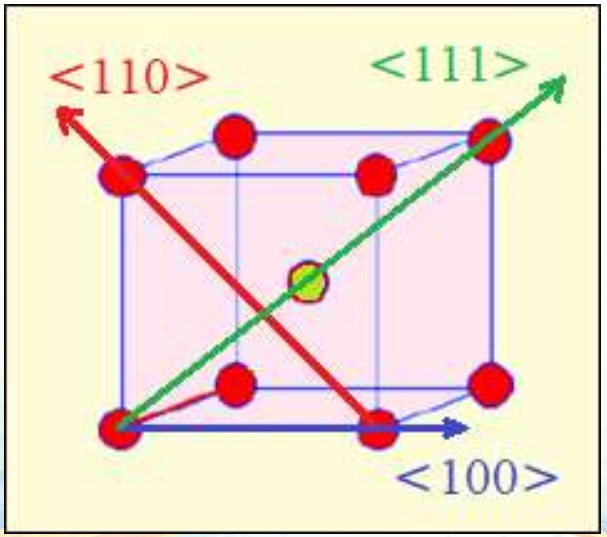
- *Anisotropic exhibiting properties with different values when measured along axes in different directions.*

- *Isotropic exhibiting properties with the same values when measured along axes in all directions.*

Anisotropy

- Different directions in a crystal have different packing.
- For instance, atoms along the edge of FCC unit cell are more separated than along the face diagonal.
- This causes anisotropy in the properties of crystals, for instance, the deformation depends on the direction in which a stress is applied.
- In some polycrystalline materials, grain orientations are random, so bulk material properties are isotropic

- *Some polycrystalline materials have grains with preferred orientations (texture), so properties are dominated by those relevant to the texture orientation and the material exhibits anisotropic properties.*
- *Properties of crystals may be different along different directions, because atomic periodicities are different.*
- *E.g. in single crystal cubic system:*

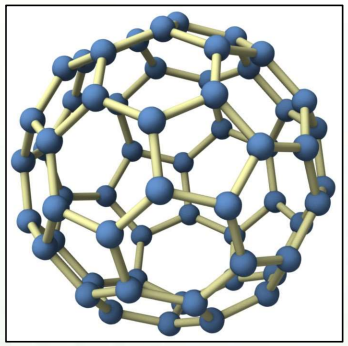


- *< 100 > Cube edges*
- *< 110 > Face diagonals*
- *< 111 > Body diagonals*

Polymorphism and Allotropy

- Some materials may exist in more than one crystal structure, this is called polymorphism.
- If the material is an elemental solid, it is called allotropy.
- Allotropy means the existence of a substance in two or more different forms in the same phase.
- An example of allotropy is carbon, which can exist as diamond, graphite, and amorphous carbon.

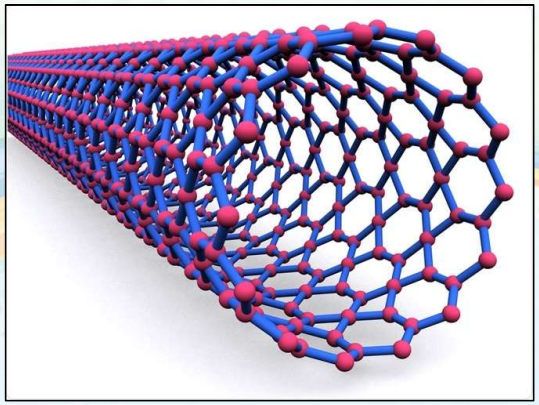
- *Pure, solid carbon occurs in three crystalline forms-diamond, graphite; and large, hollow fullerenes.*
- *Two kinds of fullerenes are shown here:*
  1. *buckminsterfullerene (Buckyball)*
  2. *carbon nanotube.*



Buckyball

Graphite

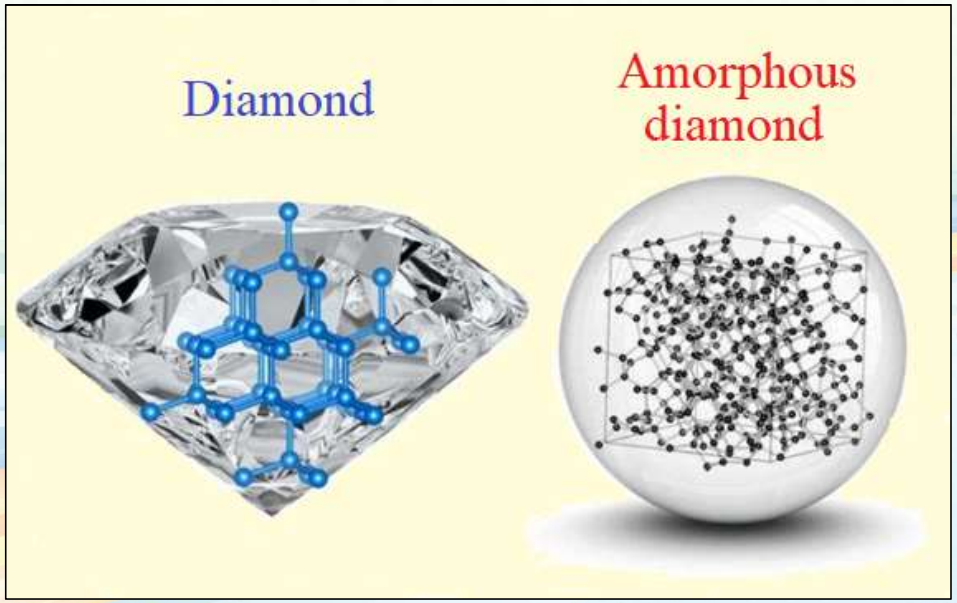
Diamond



Carbon nanotube

Non-Crystalline (Amorphous) Solids

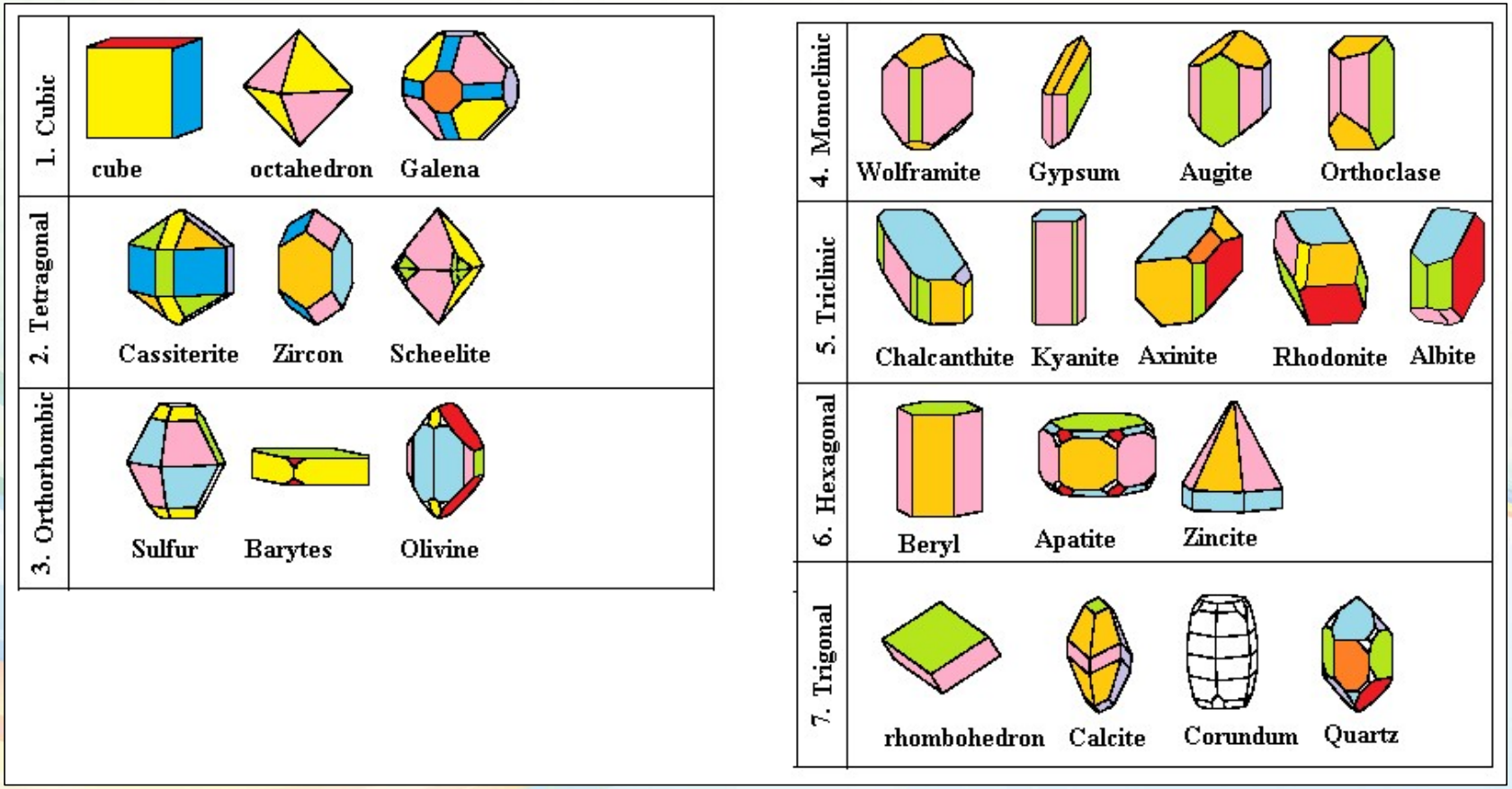
- In amorphous solids, there is no long-range order.
- But amorphous does not mean random, in many cases there is some form of short-range order.



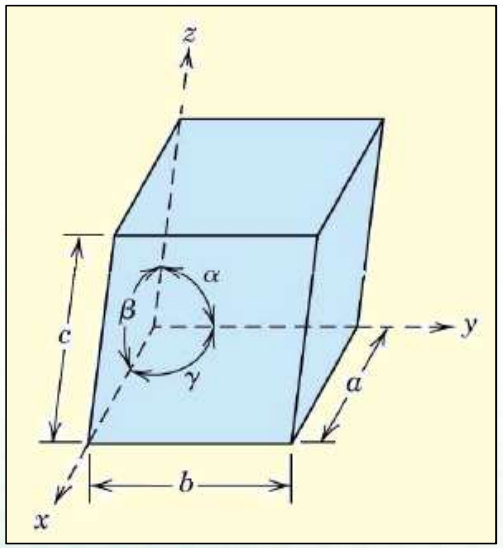
Crystallographic Points, Directions, and Planes

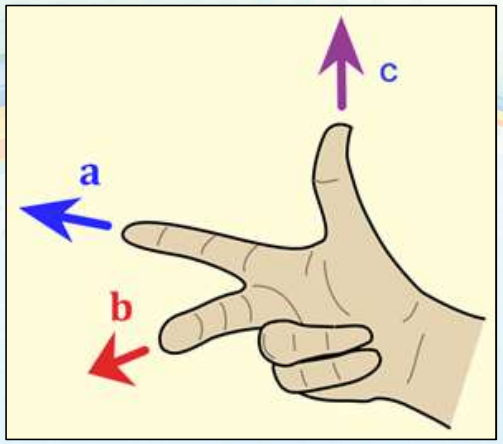
- How to define points, directions, planes, as well as linear, planar, and volume densities.
  - ✓ Points (atomic positions)
  - ✓ Vectors (defines a particular direction – plane normal)
  - ✓ Miller Indices (defines a particular plane) relation to diffraction
  - ✓ 3-indices for cubic and 4-indices notation for HCP

Symmetry Equivalent Directions



- All periodic unit cells may be described via these vectors and angles, if and only if a, b, and c define axes of a 3D coordinate system.
- Coordinate system is Right-Handed.
- We can define points, directions and planes with a "triplet" of numbers in units of a, b, and c unit cell vectors.
- For HCP we need a "quad" of numbers.

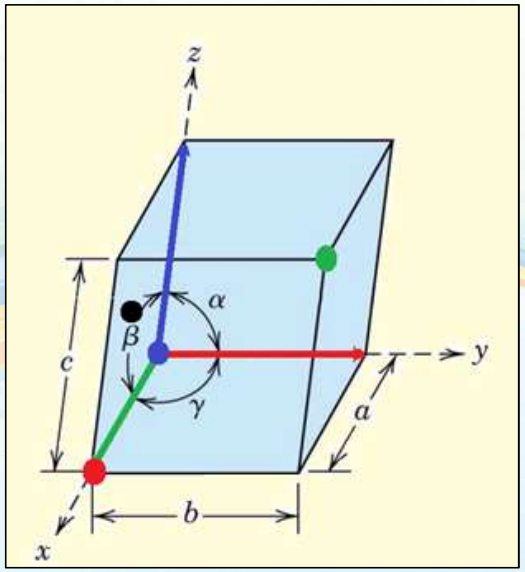




POINT Coordinates

- To define a point within a unit cell….
- Express the coordinates uvw as fractions of unit cell vectors a, b, and c (so that the axes x, y, and z do not have to be orthogonal).

	Pt. coordinate		
Point	x(a)	y(b)	z(c)
Blue	0	0	0
Red	1	0	0
Green	1	1	1
Black	1/2	0	1/2

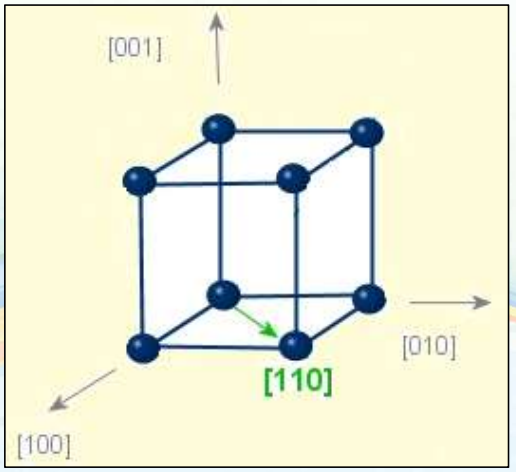


Direction Coordinates

Procedure:

1. Any line (or vector direction) is specified by 2 points.
   - ✓ The first point is, typically, at the origin (000).
2. Determine length of vector projection in each of 3 axes in units (or fractions) of a, b, and c.

X(a)	Y(b)	Z(c)
1	1	0



3. Multiply or divide by a common factor to reduce the length to the smallest integer values, u v w.
4. Enclose in square brackets: [u v w]: [110] direction.
5. Designate negative numbers by a bar $[\bar{1}\,\bar{1}\,0]$
   - ✓ Pronounced "bar 1", "bar 1", "zero" direction.
6. "Family" of [110] directions is designated as <110>.

Direction Coordinates

What is the crystallographic direction of the red arrow?

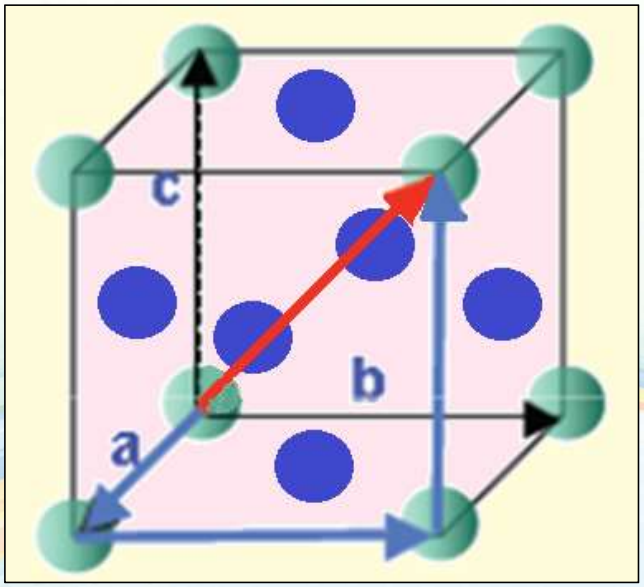
Solution:

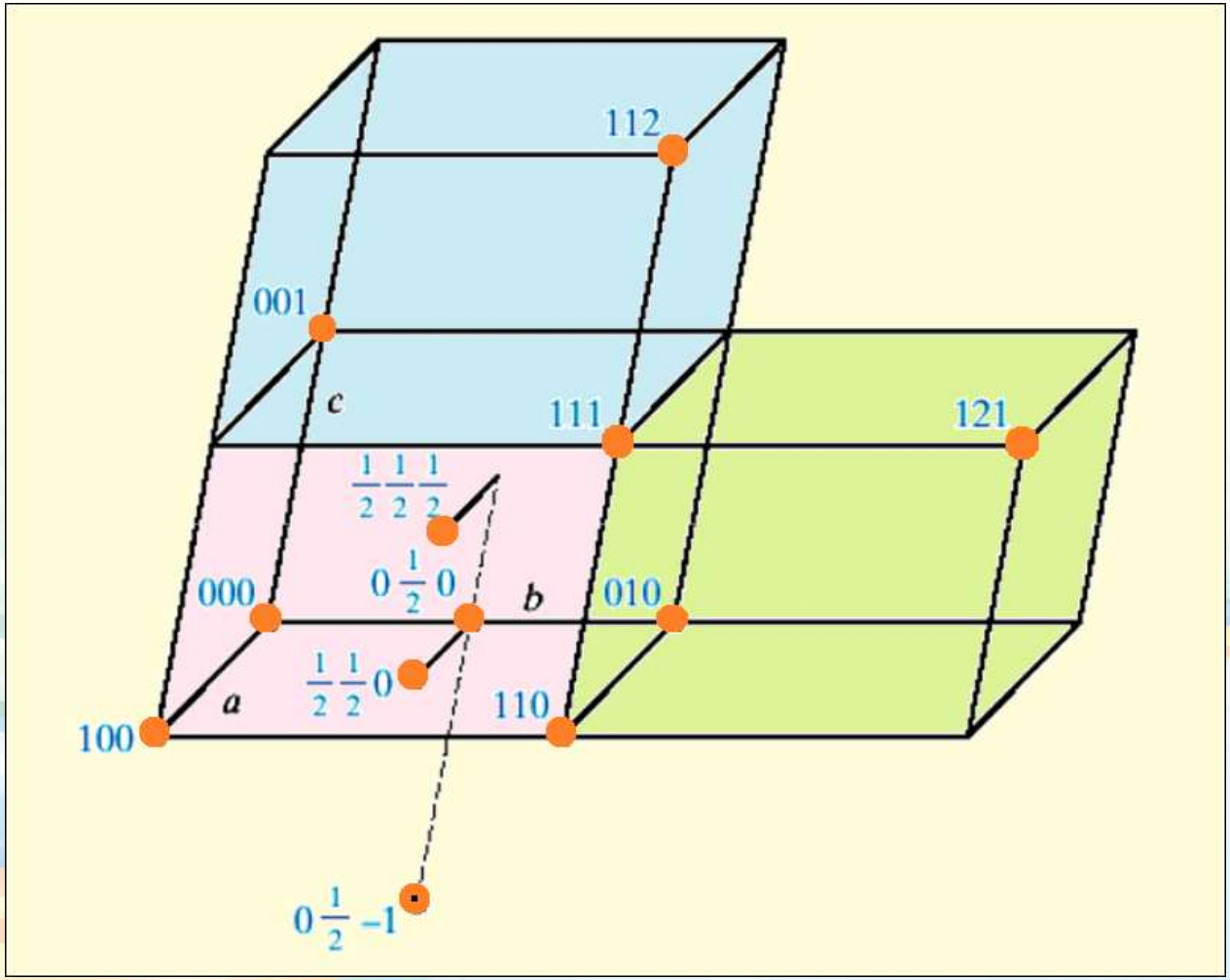
Along x: 1 a

Along y: 1 b

Along c: 1 C

Direction = [1 1 1]




112
001
c
111
121
$\frac{1}{2}\frac{1}{2}\frac{1}{2}$
000
$0\frac{1}{2}0$
b
010
$\frac{1}{2}\frac{1}{2}0$
a
110
100
$0\frac{1}{2}-1$

Point and Direction Coordinates

a) What is the lattice point given by point P?

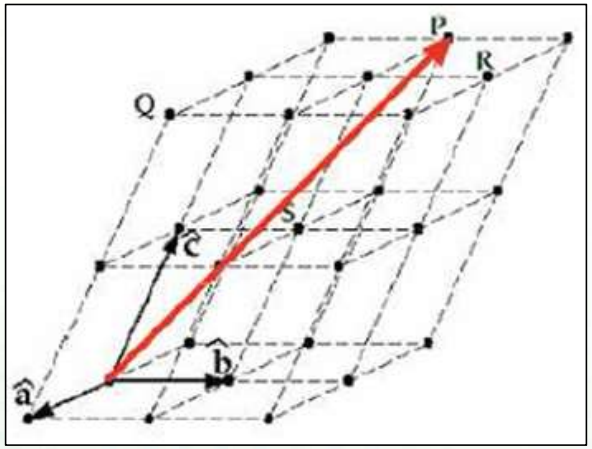
Solution:

$\bar{1}$ 1 2

b) What is the crystallographic direction for the origin to P?

Solution:

$[\bar{1}\ 1\ 2]$



c) What lattice direction does the lattice point 264 correspond?

Solution:

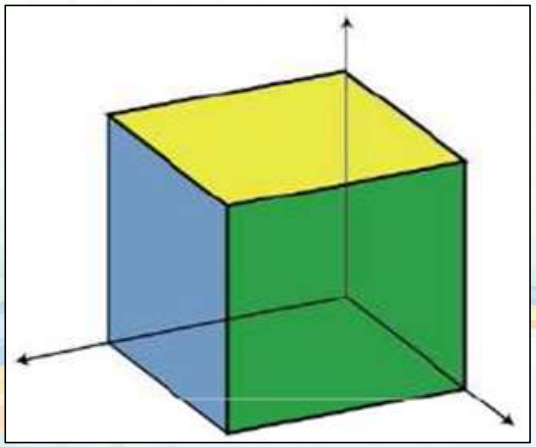
The lattice direction [1 3 2] from the origin

Symmetry Equivalent Directions

Note: for some crystal structures, different directions can be equivalent.

e.g. For cubic crystals, the directions are all equivalent by symmetry:

$[1\ 0\ 0]$, $[\bar{1}\ 0\ 0]$, $[0\ 1\ 0]$,
$[0\ \bar{1}\ 0]$, $[0\ 0\ 1]$, $[0\ 0\ \bar{1}]$

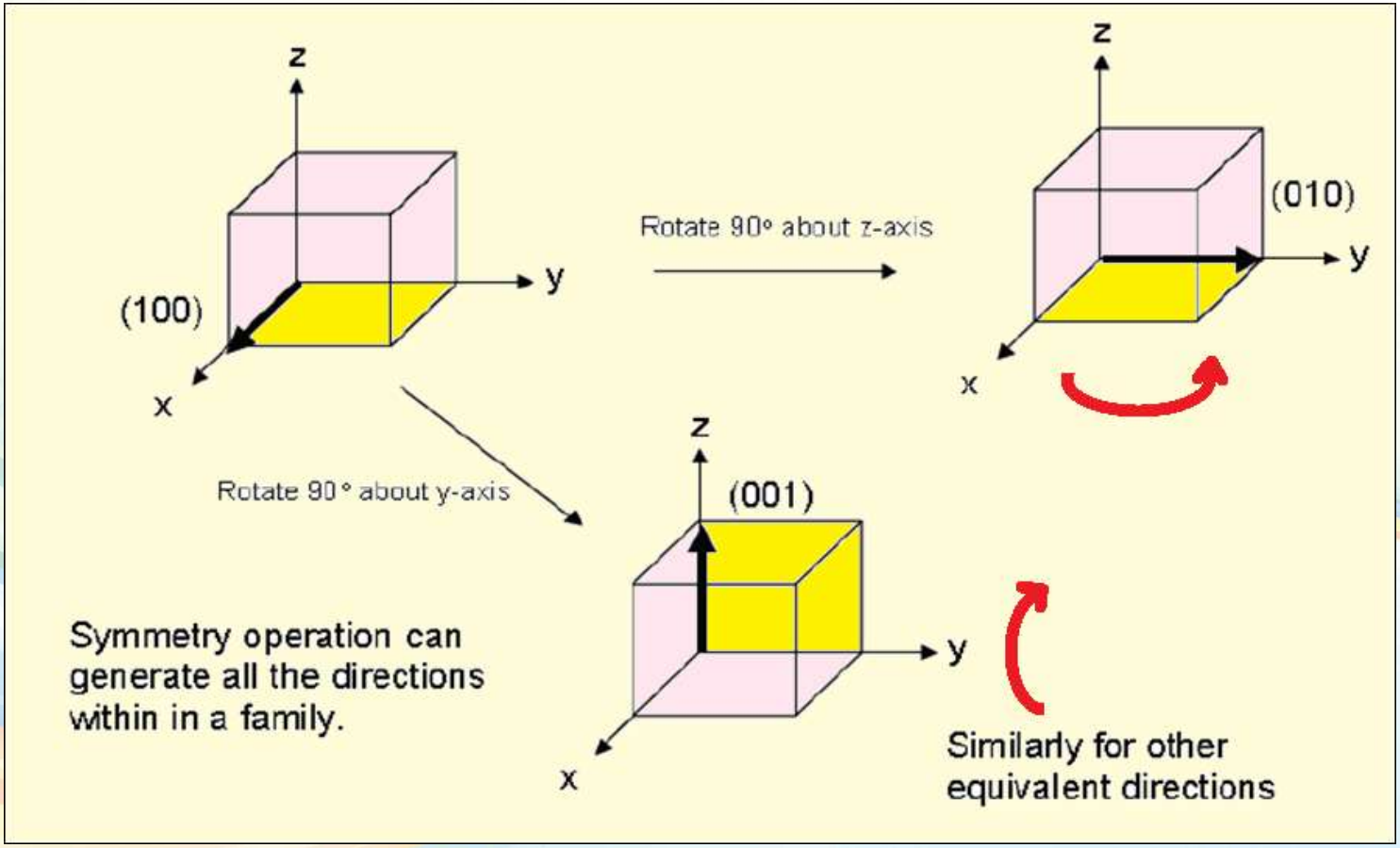


Families of crystallographic directions

e.g. $<1\ 0\ 0>$

Angled brackets denote a family of crystallographic directions

Symmetry Equivalent Directions



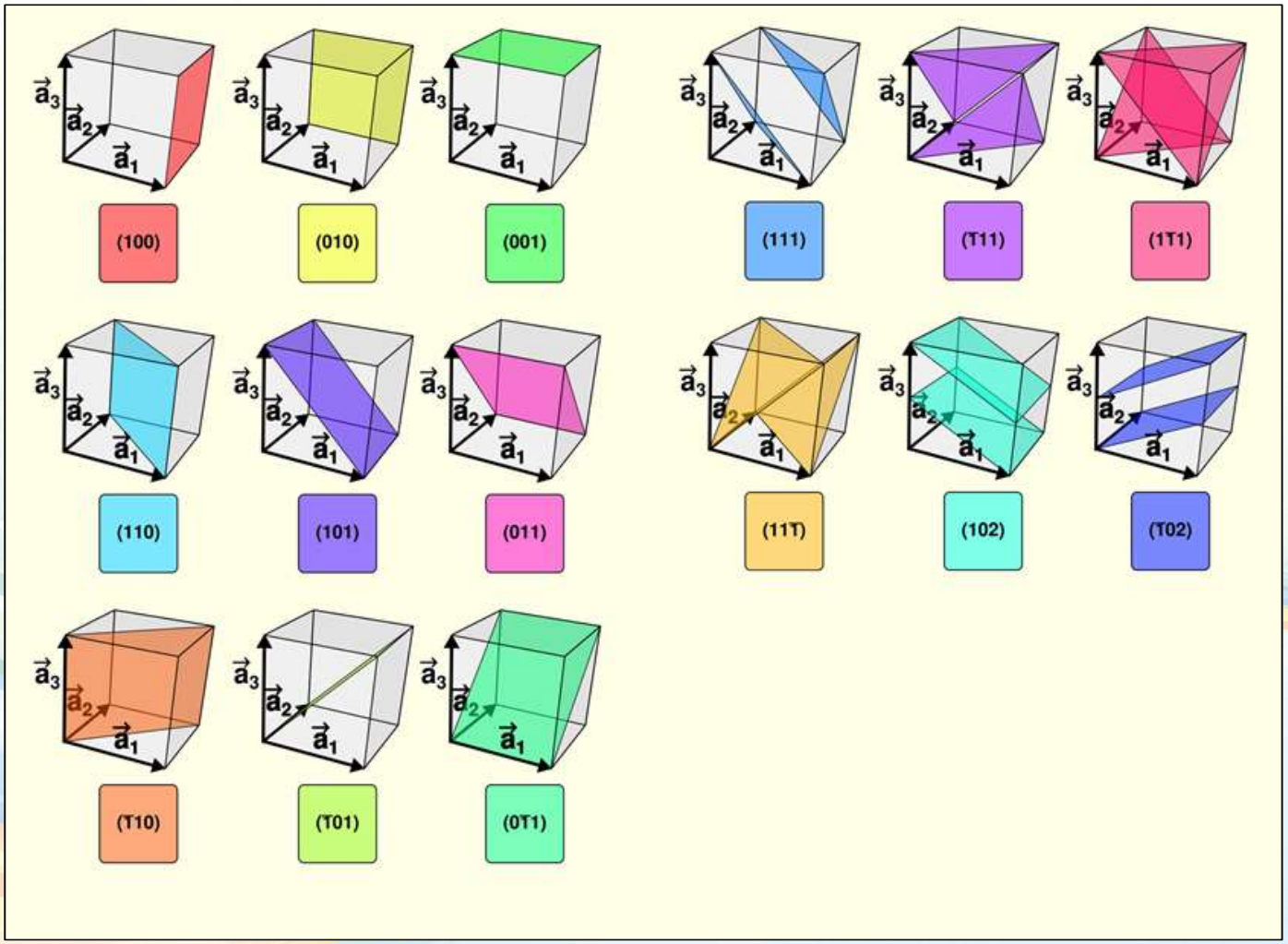
How Do We Designate Lattice Planes?

Crystallographic Planes

- Miller Indices: Reciprocals of the (three axial intercepts for a plane, cleared of fractions and common multiples.
- All parallel planes have same Miller indices.

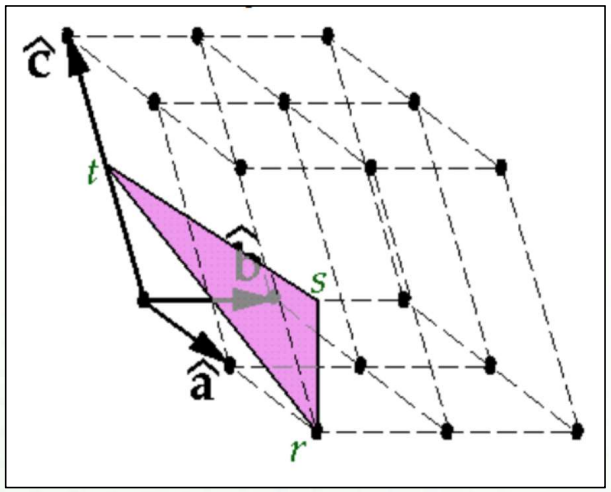
Algorithm

1. Read off intercepts of plane with axes in terms of a, b, and c.
2. Take reciprocals of intercepts.
3. Reduce to smallest integer values
4. Enclose in parentheses, no commas i.e., (h k l)


(100)
(010)
(001)
(111)
(T11)
(1T1)
(110)
(101)
(011)
(11T)
(102)
(T02)
(T10)
(T01)
(0T1)

Planes intersects axes at:

- a axis at r = 2
- b axis at s = 4/3
- c axis at r = ½



How do we symbolically designate planes in a lattice?

1. Take the reciprocal of r, s, and t.
   Here: 1/r = ½, 1/s = ¾, and 1/t = 2
2. Find the least common multiple that converts all reciprocals to integers.
   With LCM = 4, h = 4/r = 2, k = 4/s = 3, and l = 4/t = 8
3. Enclose the new triple (h, k, l) in parentheses: (2 3 8)
4. This notation is called the Miller Index.

Note 1: if a plane does not intercept an axes (i.e., it is at ∞), then you get 0.

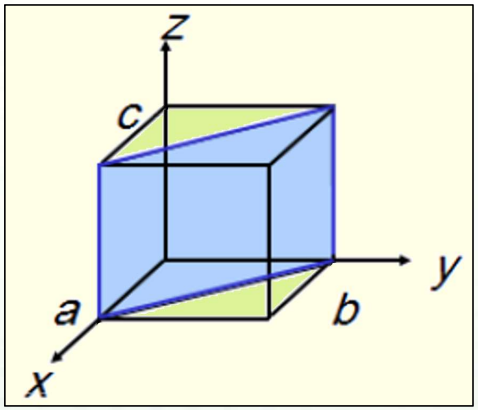
Note 2: All parallel planes at similar staggered distances have the same Miller Index.

Crystallographic Planes

Example 1

	a	b	c
Intercepts	1	1	∞
Reciprocals	1/1 1	1/1 1	1/∞ 0
Reduction	1	1	0

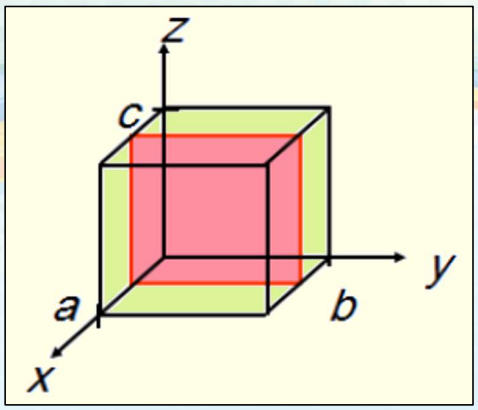
Miller Indices: (1 1 0)



Example 2

	a	b	c
Intercepts	1/2	∞	∞
Reciprocals	1/(1/2) 2	1/∞ 0	1/∞ 0
Reduction	2	0	0

Miller Indices: (2 0 0)

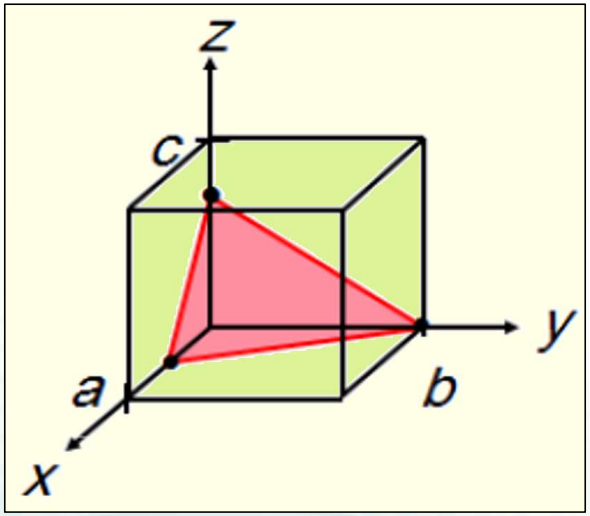


Crystallographic Planes

Example 3

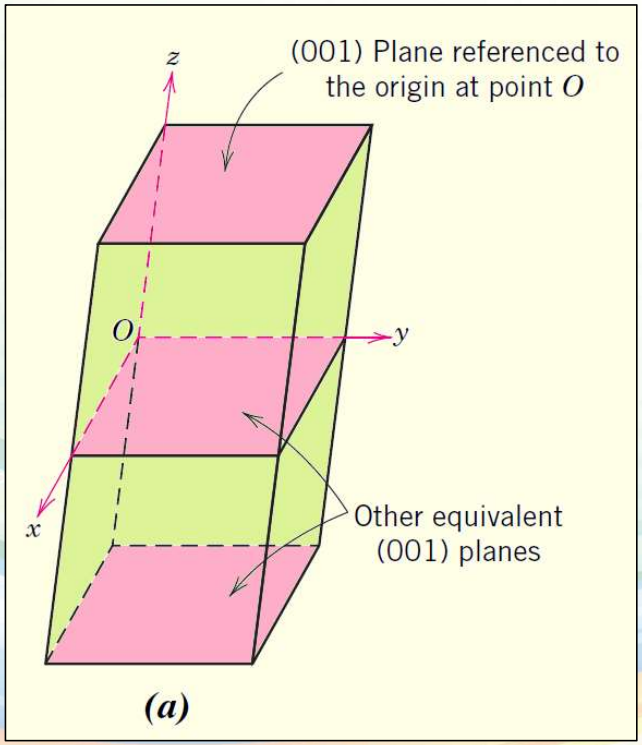
	a	b	c
Intercepts	1/2	1	3/4
Reciprocals	1/(1/2) 2	1/1 1	1/(3/4) 4/3
Reduction	6	3	4

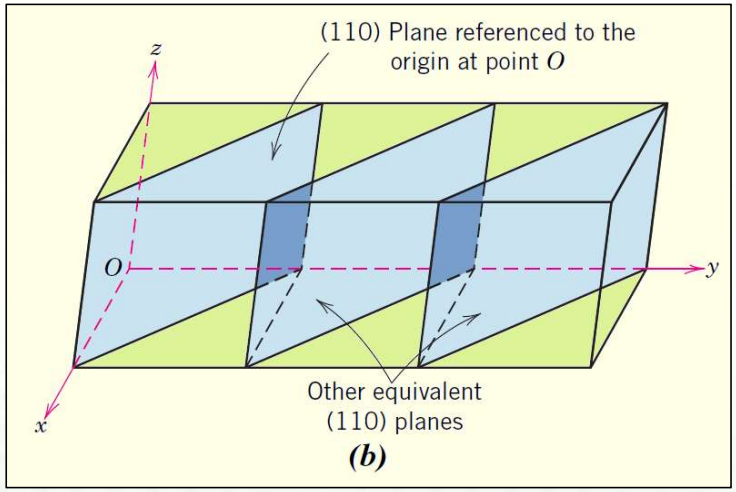
Miller Indices: (6 3 4)

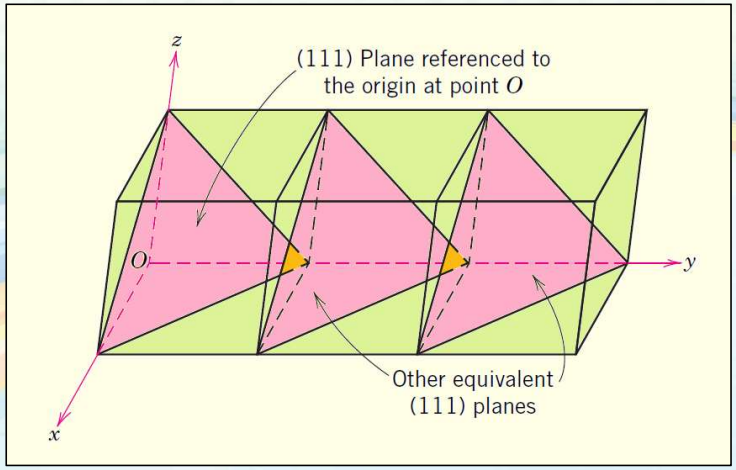


Family of Planes {h k l}

Ex: {1 0 0} = (1 0 0), (0 1 0), (0 0 1), $(\bar{1}\ 0\ 0)$, $(0\ \bar{1}\ 0)$, $(0\ 0\ \bar{1})$


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

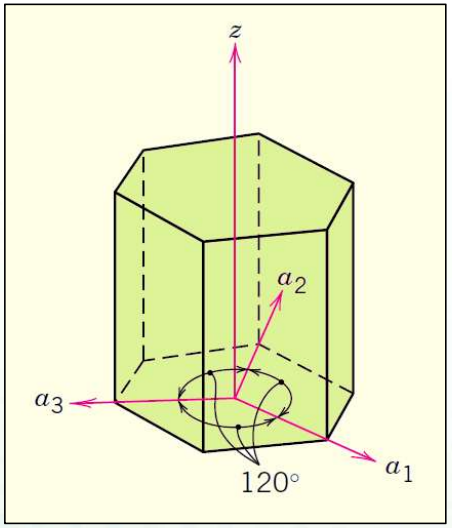

z
(110) Plane referenced to the
origin at point O
O
y
x
Other equivalent
(110) planes
(b)


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

HCP Crystallographic Directions

Algorithm

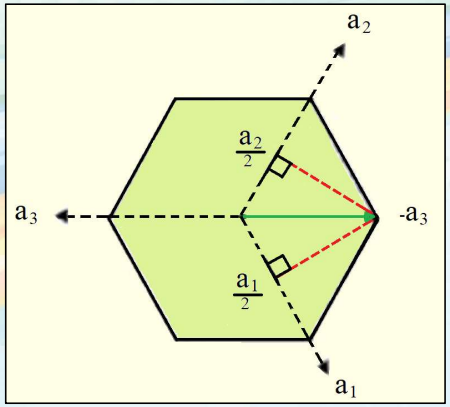
1. Vector repositioned (if necessary) to pass through origin.
2. Read off projections in terms of unit cell dimensions a_1, a_2, a_3, or c
3. Adjust to smallest integer values
4. Enclose in square brackets, no commas [u v t w].

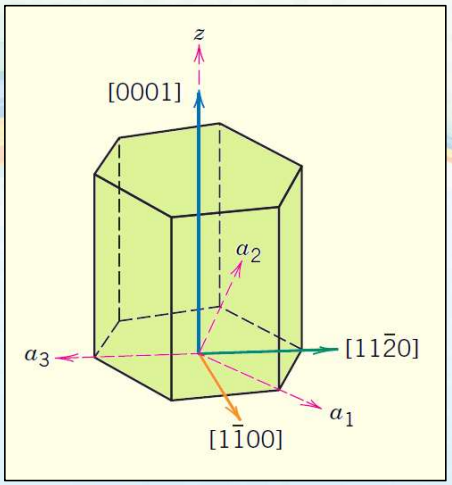


Ex:

½, ½, -1, 0 ⟹ $[1\ 1\ \bar{2}\ 0]$

Dashed red lines indicate projections onto a_1 and a_2 axes





HCP Crystallographic Directions

Hexagonal Crystals

4 parameter Miller-Bravais lattice coordinates are related to the direction indices (i.e., $\acute{u}\ \acute{v}\ \acute{w}$) as follows.

$$[\acute{u}\ \acute{v}\ \acute{w}] \rightarrow [u\ v\ t\ w]$$

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

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

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

$$w = \acute{w}$$

$[\acute{u}\ \acute{v}\ \acute{w}]=[1\ \ 1\ \ 0]$

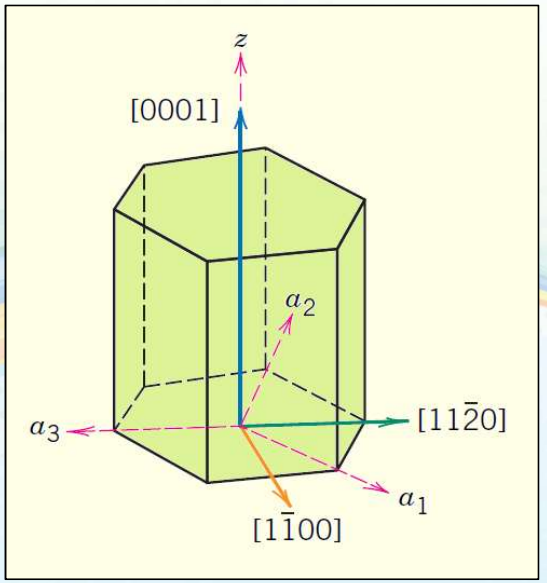
$$u = \frac{1}{3}(2 \times 1 - 1) = \frac{1}{3}$$

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

$$t = -\left(\frac{1}{3} + \frac{1}{3}\right) = -\frac{2}{3}$$

$$w = 0$$

$$\left[\frac{1}{3}\ \ \frac{1}{3}\ \ \frac{-2}{3}\ \ 0\right] = [1\ 1\ \bar{2}\ 0]$$



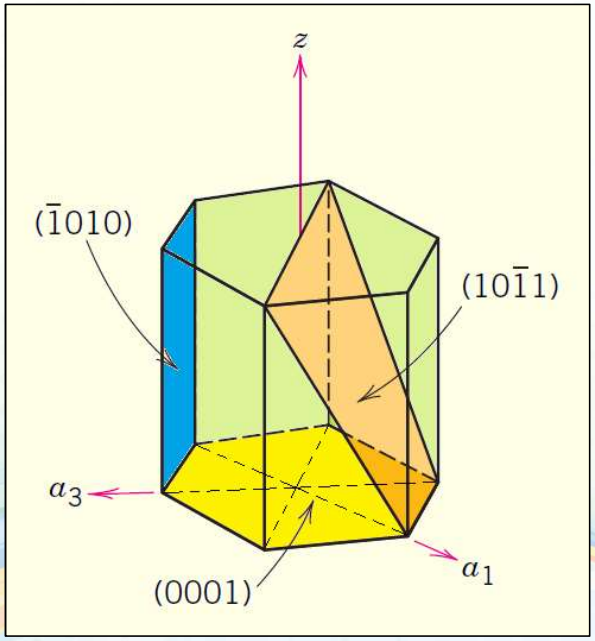
HCP Crystallographic Planes

- In hexagonal unit cells the same idea is used:

Example 3

	a_1	a_2	a_3	c
Intercepts	1	∞	-1	1
Reciprocals	1 1	1/∞ 0	-1 -1	1 1
Reduction	1	0	-1	1

Miller-Bravais Indices: $(1\ 0\ \bar{1}\ 1)$



Linear Density

$$Linear\ Density\ of\ Atoms = LD = \frac{Number\ of\ atoms\ centered\ on}{Unit\ length\ of\ direction\ vector}$$

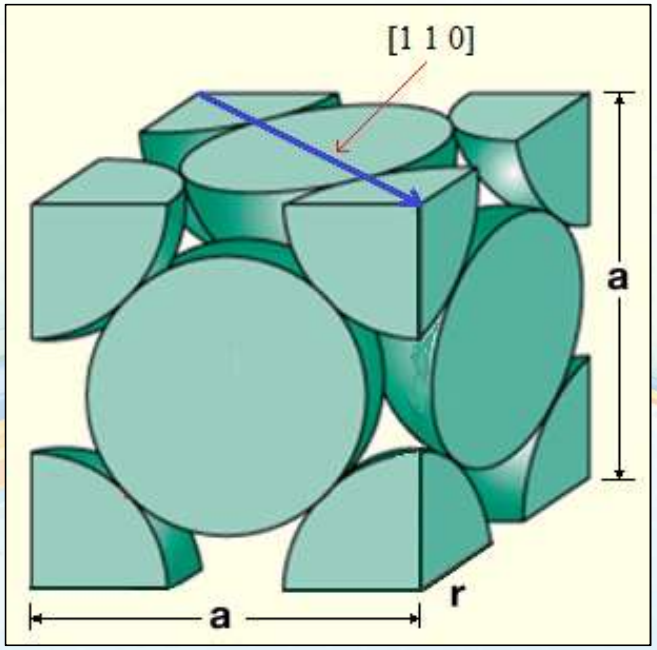
Example:

Calculate the linear density of Al in [1 1 0] direction. Al atomic radius = 0.143 nm

We know:

- Number of atoms centered = 2
- Unit length of direction vector = 4r

$$LD = \frac{2}{4 \times 0.143} = 3.4965\ nm^{-1}$$



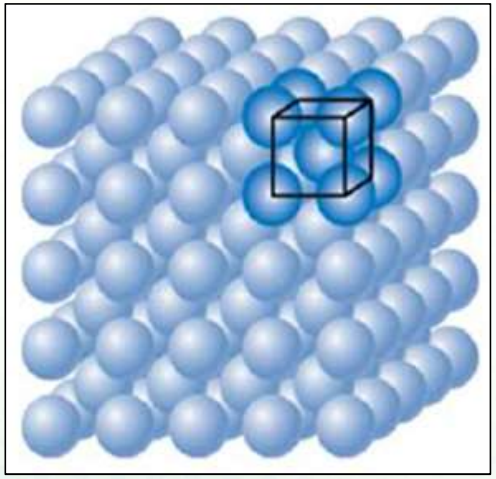
Planar Density

Example:

Calculate the Planar density of (1 0 0) Iron.

At T 912 oC iron has the BCC structure.

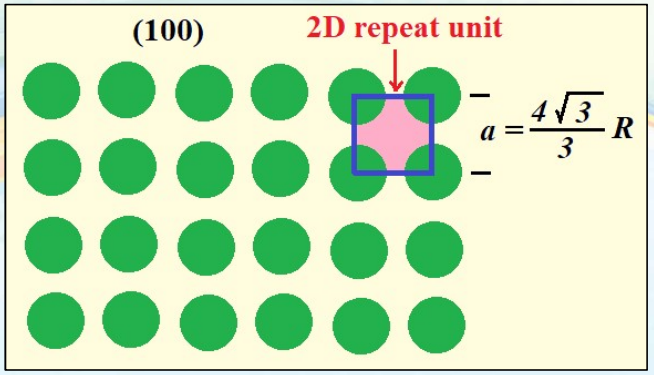
- Radius of iron R = 0.1241 nm
- Number of atoms in the plane = 1
- Area of plane = a^2



$$Plamar\ Density = \frac{Number\ of\ atoms\ in\ the\ plane}{Area\ of\ the\ plane}$$

$$Plamar\ Density = \frac{1}{a^2} = \frac{1}{\left(\frac{4\sqrt{3}}{3}R\right)^2}$$

$$12.1\ \frac{atoms}{nm^2} = 1.2 \times 10^{19}\ \frac{atoms}{m^2}$$

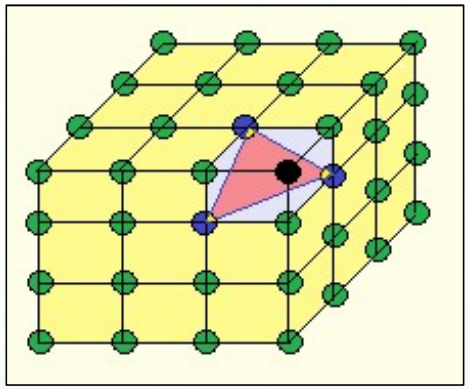


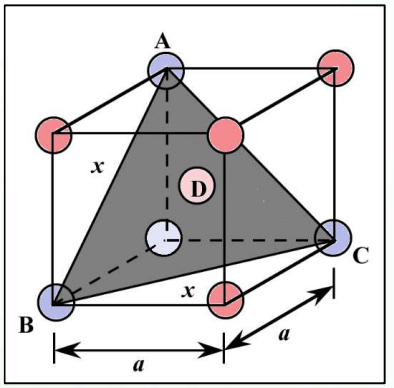
Planar Density

Excersise:

Calculate the planar density of (1 1 1) iron.

- Radius of iron $R = 0.1241\ nm$
- Number of atoms in the plane = 0.5



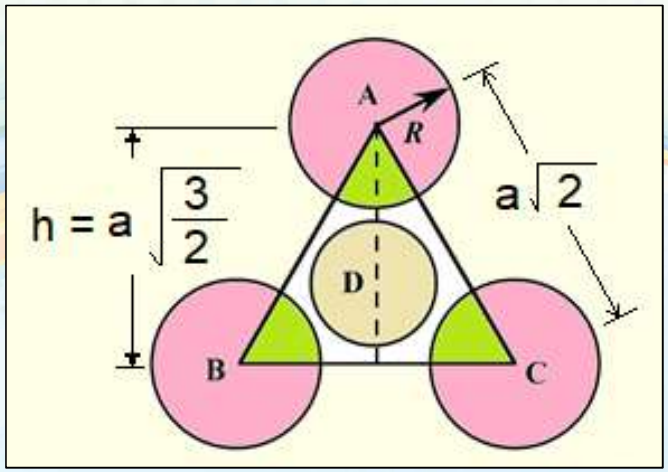


- Area of plane $= \frac{\sqrt{3}}{2}a^2$

$$= \frac{\sqrt{3}}{2}\left(\frac{4}{\sqrt{3}}R\right)^2 = \frac{8}{\sqrt{3}}R^2$$

$$Plamar\ Density = \frac{0.5}{area} = \frac{0.5}{\frac{8}{\sqrt{3}}R^2}$$

$$= 0.703 \times 10^{19}\ \frac{atoms}{m^2}$$



Designating Lattice Planes

Why are planes in a lattice important?

A. Determining crystal structure:

- Diffraction methods measure the distance between parallel lattice planes of atoms. This information is used to determine the lattice parameters in a crystal.
- Diffraction methods also measure the angles between lattice planes.

B. Plastic deformation

- Plastic deformation in metals occurs by the slip of atoms past each other in the crystal.
- This slip tends to occur preferentially along specific crystal-dependent planes.

B. Transport Properties

In certain materials, atomic structure in some planes causes the transport of electrons and/or heat to be particularly rapid in that plane, and relatively slow in other planes.

Example:

Graphite: heat conduction is more in sp^2-bonded plane.