Engineering Physics:

Physics of Materials: Crystal Structure

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Crystal Physics

Electronic Materials

- The goal of electronic materials is to generate and control the flow of an electrical current.

- Electronic materials include:

  1. <u>Conductors</u>: have low resistance which allows electrical current flow

  2. <u>Insulators</u>: have high resistance which suppresses electrical current flow

  3. <u>Semiconductors</u>: can allow or suppress electrical current flow
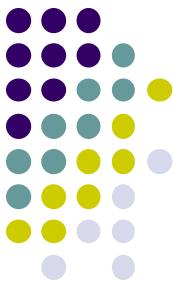
Electrical Resistivity and Conductivity of Selected Materials at 293 K

Table 11.1 **Electrical Resistivity and Conductivity of Selected Materials at 293 K**

| Material	Resistivity $(\Omega \cdot m)$	Conductivity $(\Omega^{-1} \cdot m^{-1})$
Metals		
Silver	1.59×10^{-8}	6.29×10^{7}
Copper	1.72×10^{-8}	5.81×10^{7}
Gold	2.44×10^{-8}	4.10×10^{7}
Aluminum	2.82×10^{-8}	3.55×10^{7}
Tungsten	5.6×10^{-8}	1.8×10^{7}
Platinum	1.1×10^{-7}	9.1×10^{6}
Lead	2.2×10^{-7}	4.5×10^{6}
Alloys		
Constantan	4.9×10^{-7}	2.0×10^{6}
Nichrome	1.5×10^{-6}	6.7×10^{5}
Semiconductors		
Carbon	3.5×10^{-5}	2.9×10^{4}
Germanium	0.46	2.2
Silicon	640	1.6×10^{-3}
Insulators		
Wood	10^{8}–10^{11}	10^{-8}–10^{-11}
Rubber	10^{13}	10^{-13}
Amber	5×10^{14}	2×10^{-15}
Glass	10^{10}–10^{14}	10^{-10}–10^{-14}
Quartz (fused)	7.5×10^{17}	1.3×10^{-18}
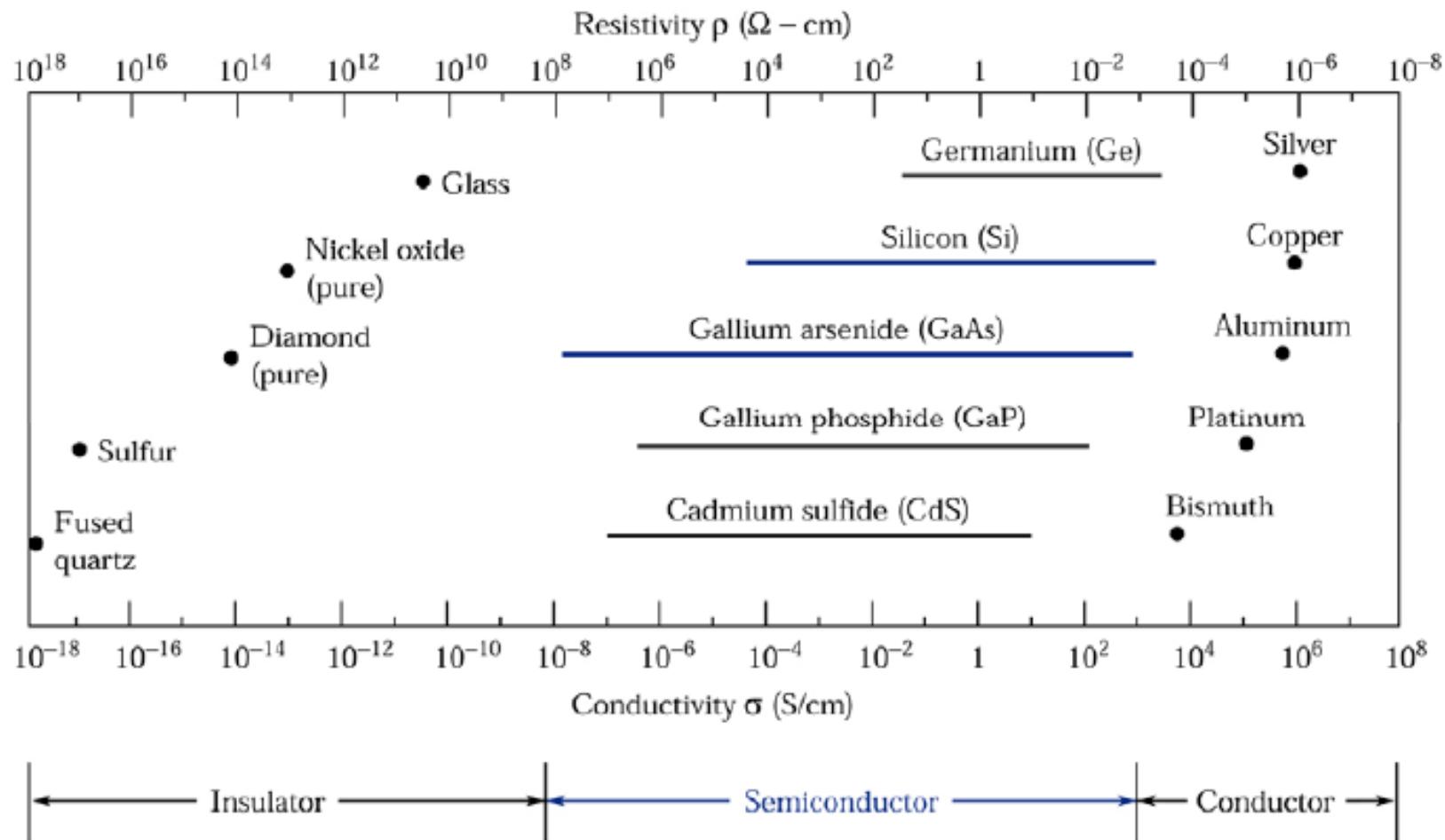
# Reviewing the previous table reveals that:

- The electrical conductivity at room temperature is quite different for each of these three kinds of solids

  - **Metals and alloys** have the highest conductivities

  - followed by **semiconductors**

  - and then by **insulators**

Semiconductor material –
conductivities for insulators, semiconductors, and conductors.

Semiconductor Conduction

- The **free-electron** model from Physics does not apply to semiconductors and insulators, since these materials simply lack enough free electrons to conduct in a free-electron mode.

  There is a different conduction mechanism for semiconductors than for normal conductors.

Resistivity vs. Temperature
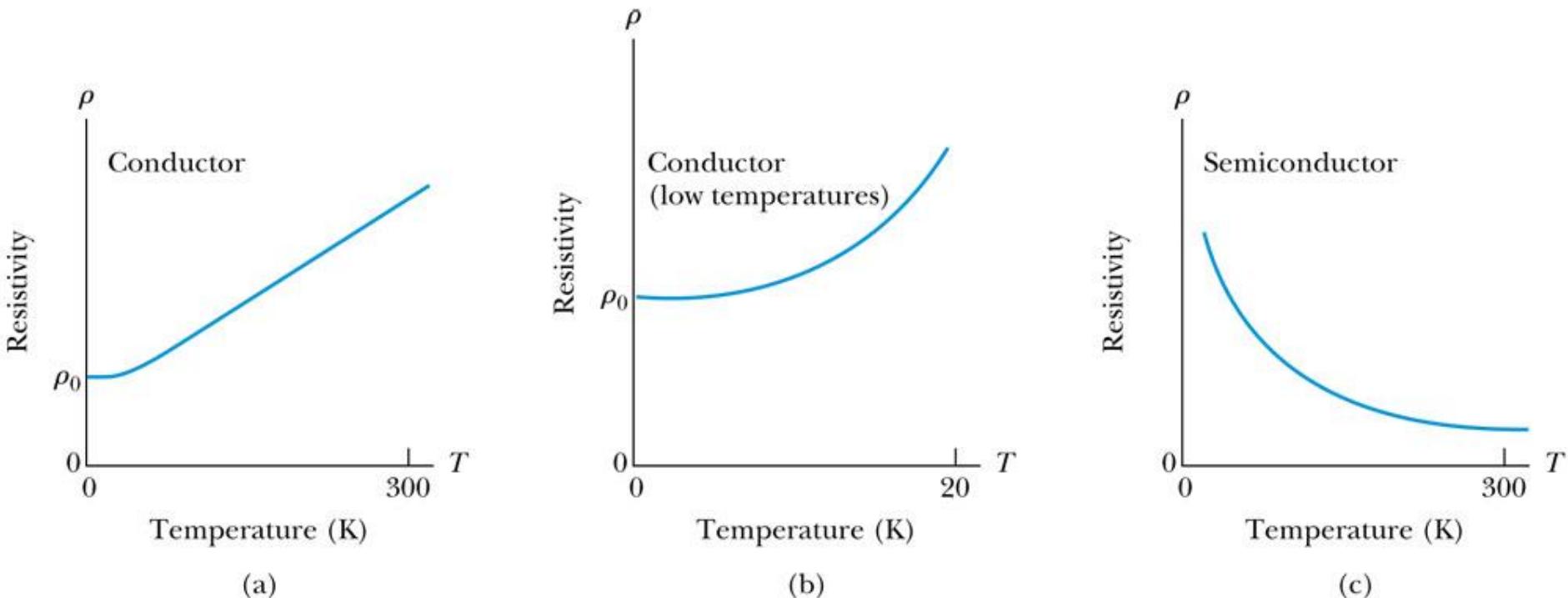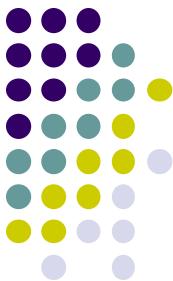
Figure 11.1: (a) Resistivity versus temperature for a typical conductor. Notice the linear rise in resistivity with increasing temperature at all but very low temperatures. (b) Resistivity versus temperature for a typical conductor at very low temperatures. Notice that the curve flattens and approaches a nonzero resistance as $T \to 0$. (c) Resistivity versus temperature for a typical semiconductor. The resistivity increases dramatically as $T \to 0$.

Resistance Effects of Doping
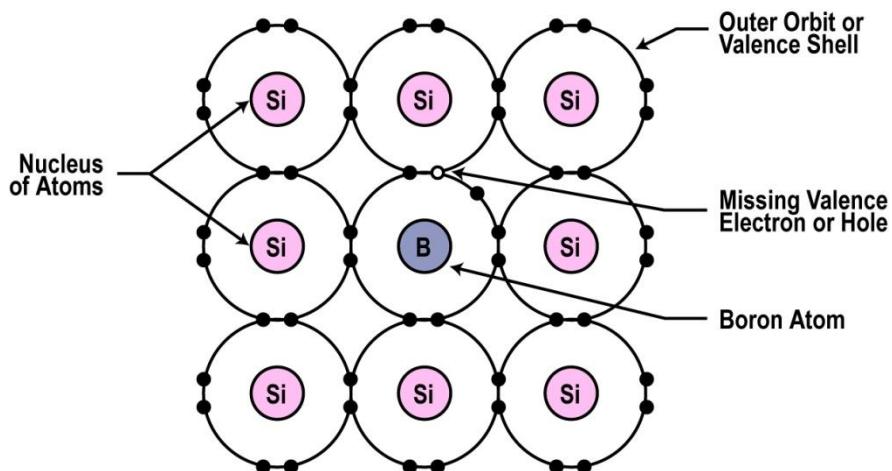
- If you use lots of arsenic atoms for doping, there will be lots of extra electrons so the resistance of the material will be low and current will flow freely.

- If you use only a few boron atoms, there will be fewer free electrons so the resistance will be high and less current will flow.

- By controlling the doping amount, virtually any resistance can be achieved.

A presentation of eSyst.org

Another Way to Dope

- You can also <u>dope</u> a semiconductor material with an atom such as boron <u>that has only 3 valence electrons</u>.
- The 3 electrons in the outer orbit do form covalent bonds with its neighboring semiconductor atoms as before. But <u>one electron is missing from the bond</u>.
- <u>This place where a fourth electron should be</u> is referred to as a <u>hole</u>.
- The hole assumes a positive charge so it can attract electrons from some other source.
- <u>Holes</u> become a type of current carrier like the electron to <u>support current flow</u>.

Outer Orbit or Valence Shell

Nucleus of Atoms

Si Si Si

Si B Si

Si Si Si

Missing Valence Electron or Hole

Boron Atom

A presentation of eSyst.org
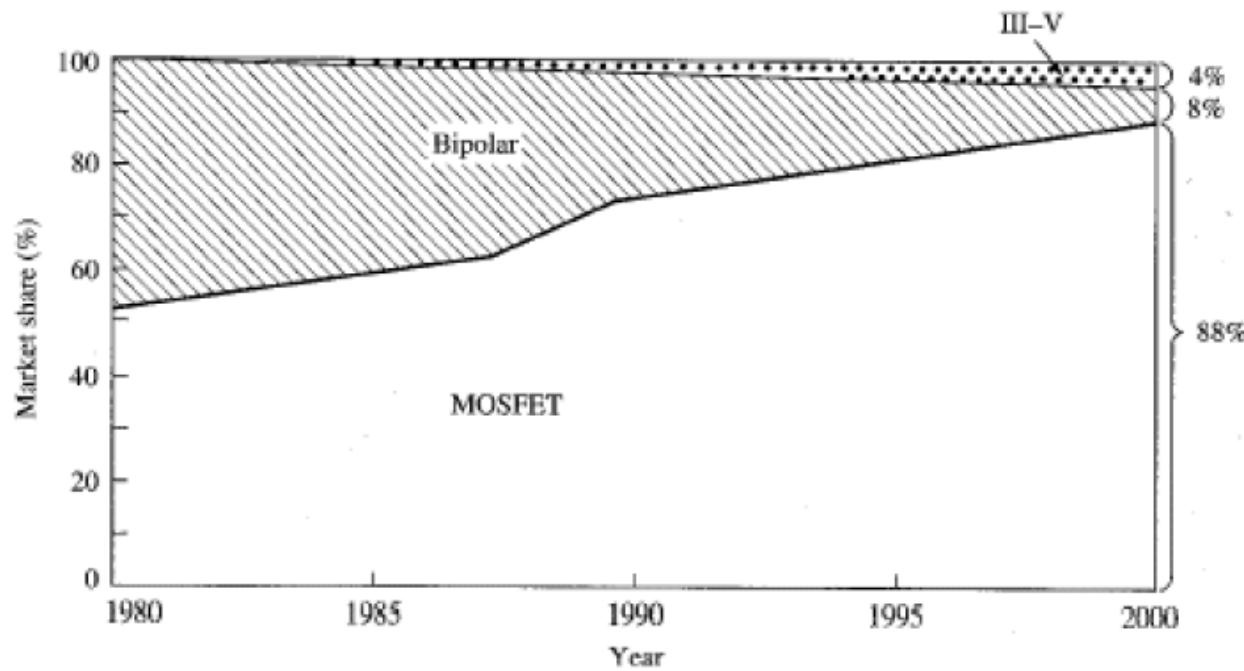
1.4 Electronic Materials

More than 95% of the electronic devices are based on silicon (Si) technology. Therefore, silicon is the most important material in semiconductor industry. Most of the electronic products like microprocessors or memory products are based on silicon technology. Alternative materials like gallium arsenide or germanium are used for specific applications, like light emitting diodes or ultra high speed electronics.

Nowadays the most important electronic device is the Metal oxide semiconductor field effect transistor (MOSFET). The MOSFET is closely related to Digital Electronics. If it comes to the realization of digital electronics the MOS transistor is the electronic device of choice. Bipolar transistors are mainly used in the area of analog electronics. Throughout the last 20 years we have seen a trend from analog to digital electronics. However, there is still (and will be) a need for analog electronics.
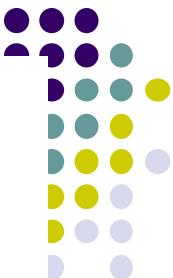
1.4 Electronic Materials
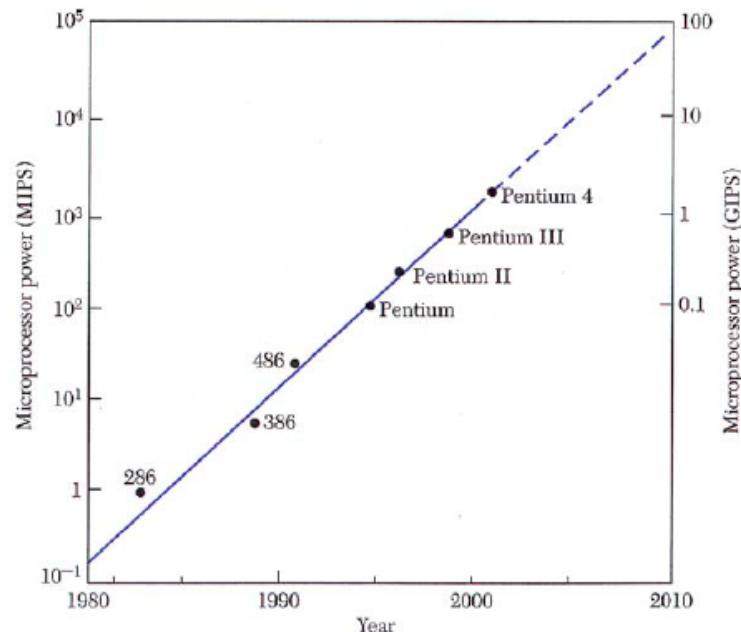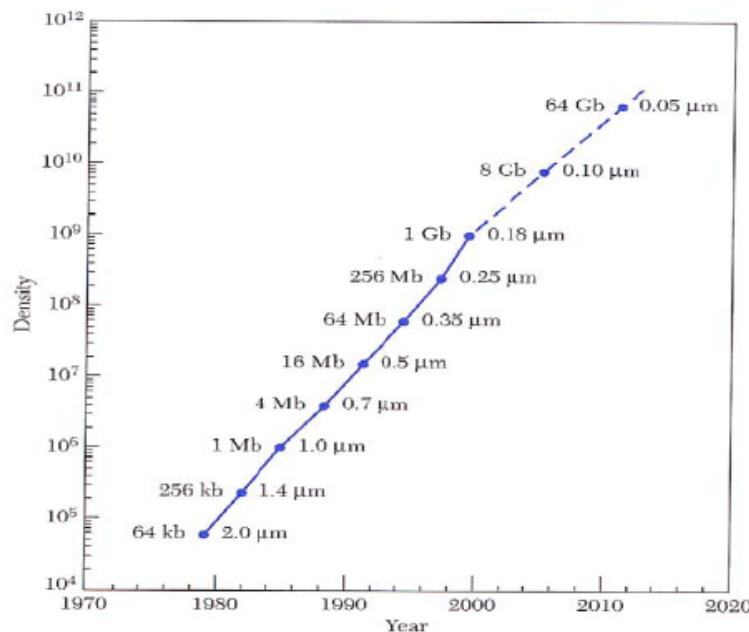
Market share of different electronic devices.

Interestingly the first transistors and the first integrated circuits were bipolar devices. Initially MOS technology had only an incremental advantage over bipolar technology. III-V technology (including materials like gallium arsenide) is of main interest in the area of optoelectronic devices like light emitting diodes.

1.5 The silicon roadmap
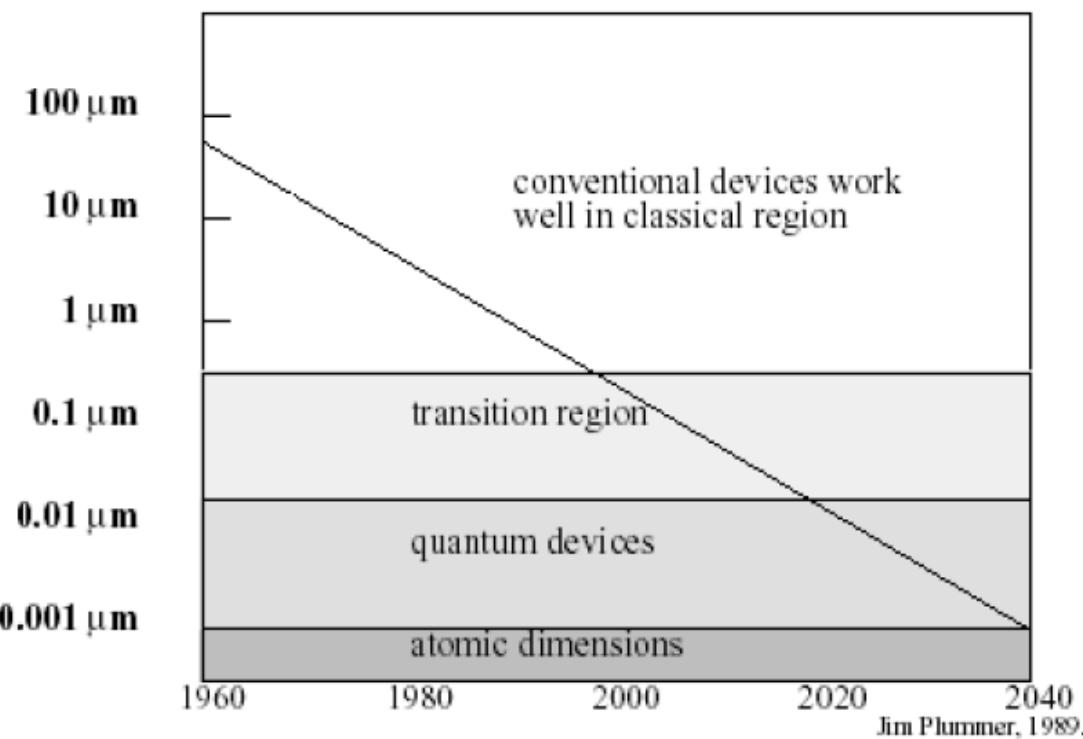
Exponential increase of the memory size (dyanmic random access memory, DRAM) and microprocessor power over time. The curves are kown as „Moore's law".

Ref.: M.S. Sze, Semiconductor Devices

1.6 What's next? (Predictions and Outlooks)

What is beyond CMOS (Complementary metal oxide semiconductor) and MOSFET (metal oxide semiconductor field effect transistors)!

Jim Plummer, 1989.
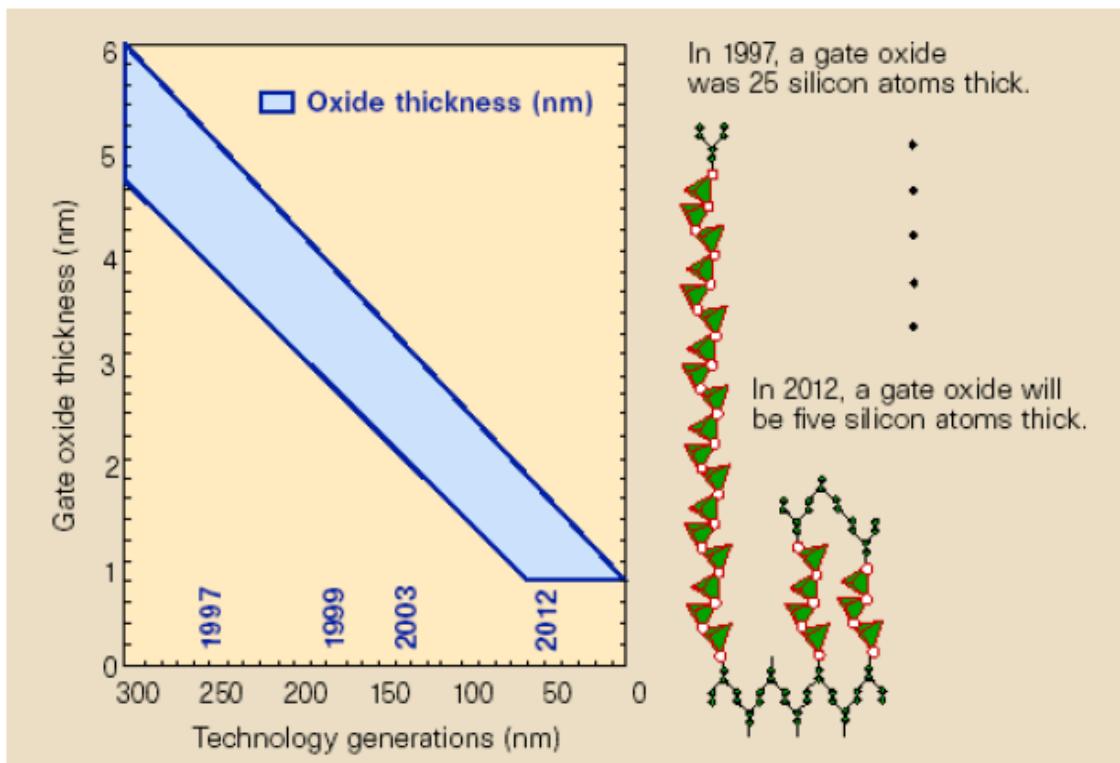
Devices are getting smaller and smaller. Will electronic devices reach quantum or even atomic dimensions?

What principles will they operate on?

1.6.1 Silicon electronics

What is beyond CMOS (Complementary metal oxide semiconductor) and MOSFET (metal oxide semiconductor field effect transistors)!

In 1997, a gate oxide was 25 silicon atoms thick.

In 2012, a gate oxide will be five silicon atoms thick.

Gate oxide thickness of metal oxide semi-conductor field effect transistors.

1.6.2 Nanotechnology!

Increasing the control over material structures of nanoscale size 0.1nm to100nm.

Top-down Approach towards Nanotechnology:
Fabrication and realization of electronic devices from macroscopic down to nanoscopic scale by a step-by-step improvement of existing technologies:
e.g. lithography in microelectronics.

Bottom-up Approach towards Nanotechnology:
Bottom-up refers to synthesis from individual molecules or atoms

The following mechanism are used to build device structures:
- Surface tension, strain, hydrophilic/hydrophobic
- Selective growth
- Supramolecular chemistry
- Fluidic self-assembly

While traditional chemistry focuses on covalent bond, superamolecular chemistry examines the weaker and reversible noncovalent interaction like hydrogen bonding, hydrophobic forces, van der waals forces, pi-pi interaction etc…

Is a new technique, which makes possible the integration of devices fabricated using dissimilar materials and processes

Classification of Materials
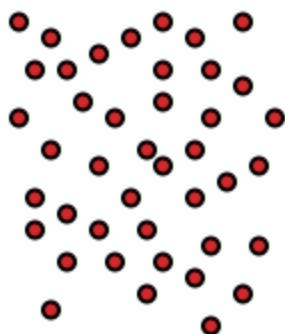

AMORPHOUS STATE
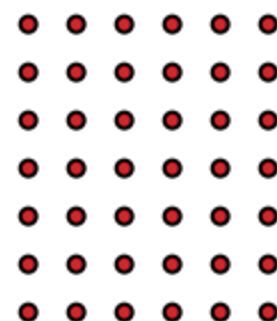
CRYSTALLINE STATE
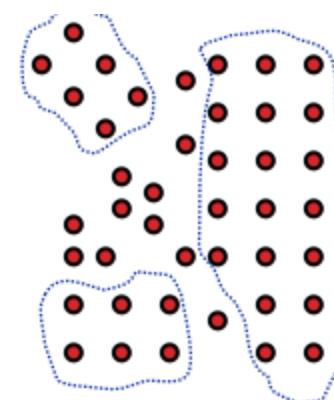
**POLYCRYSTALLINE STATE**

AMORPHOUS STATE
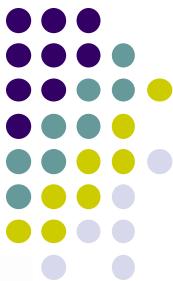
CRYSTALLINE STATE
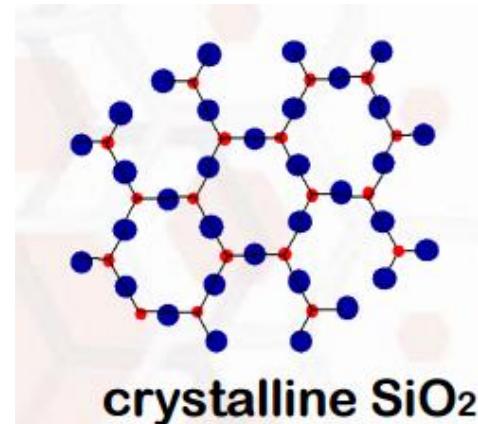
POLYCRYSTALLINE STATE

Materials and Packing
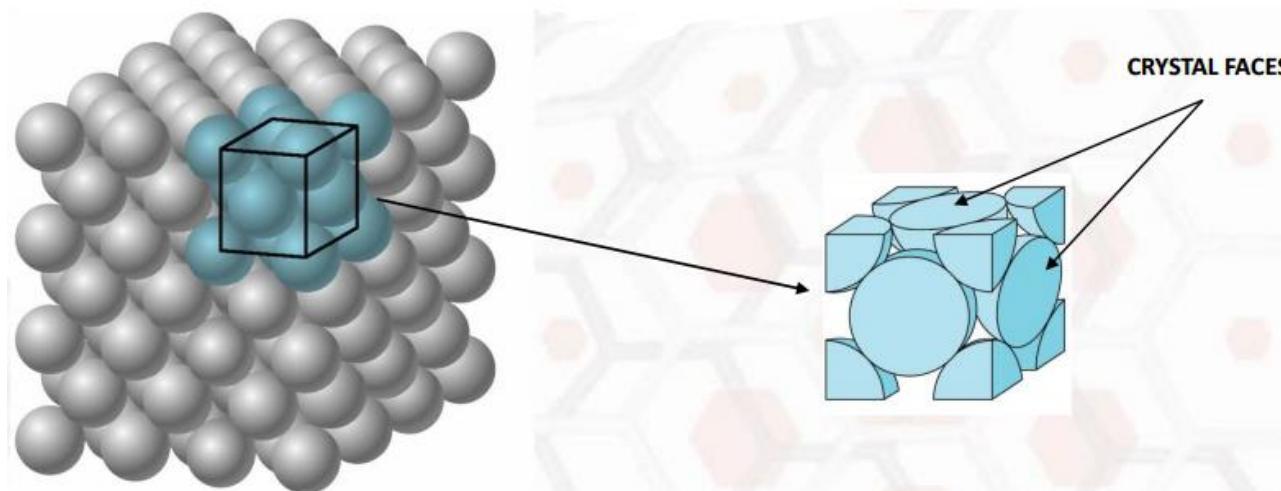
- Crystalline materials...
  - atoms pack in periodic, 3D arrays .
  - typical of: -metals ,many ceramics ,some polymers

- Non-crystalline materials...
  - atoms have no periodic packing
 - occurs for: complex structures.

  "Amorphous "= Non crystalline

crystalline SiO₂

·Si   • Oxygen

Non-crystalline SiO₂

Crystal

CRYSTAL FACES

- A **crystal** or **crystalline solid** is a solid material whose constituents (such as atoms, molecules, or ions) are arranged in a highly ordered microscopic structure, forming a crystal lattice that extends in all directions.

"A CRYSTAL is any solid material in which the component atoms are arranged in a definite pattern"

Concepts of Crystal Structure: Basis and Lattice

- A crystal lattice can always be constructed by the repetition of a fundamental set of translational vectors in real space a, b, and c, i.e., any point in the lattice can be written as:

$$r = n_1 a + n_2 b + n_3 c$$
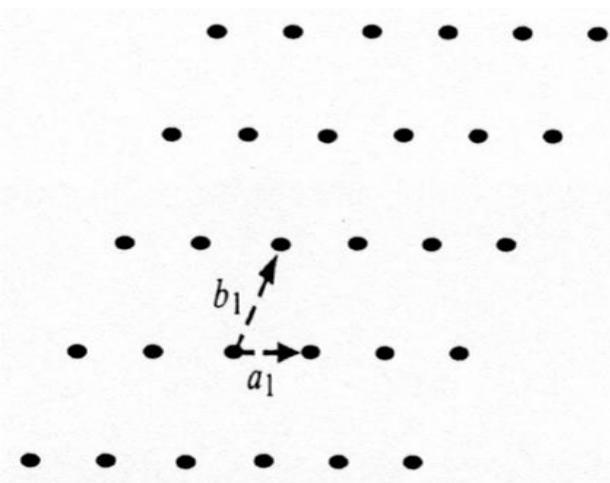
- Such a lattice is called a **Bravais lattice**. The translational vectors, a, b, and c are the primitive vectors.

Concepts of Crystal Structure: Basis and Lattice
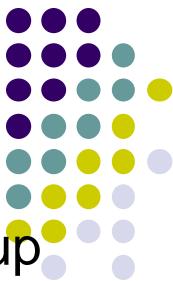
A representative unit, or group of atoms in single crystal materials is repeated at regular intervals in each of the three dimensions. The periodic arrangement of the unit or group in the crystal is called the **lattice**. Each unit or group can be represented by a dot, which is called a lattice point.

Single crystal lattices have translational symmetries (assuming each crystal is infinitely large in space). They can be characterized by three noncolinear directions. These translation directions need not be perpendicular.

# Concepts of Crystal Structure: Basis and Lattice
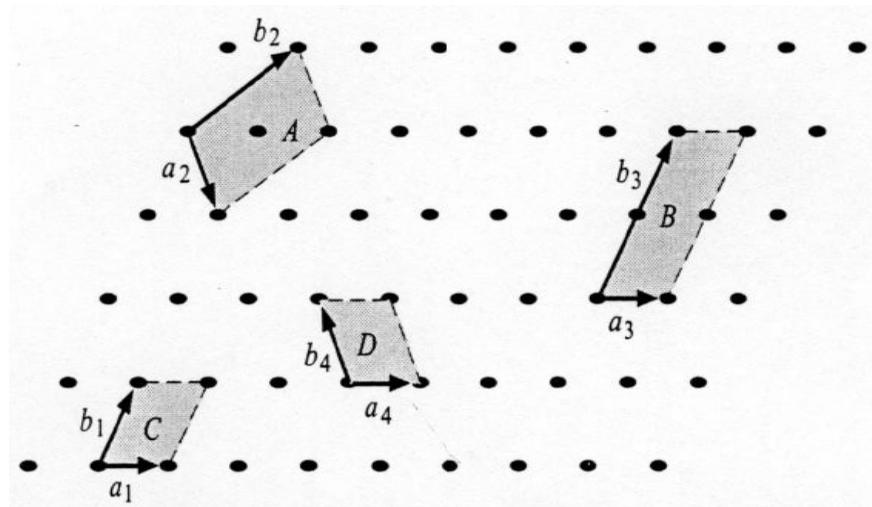
Because a three-dimensional lattice is a periodic repetition of a group of atoms, we need consider only a fundamental unit that is being repeated. A **unit cell** is a small volume of the crystal that can be used to reproduce the entire crystal.

A unit cell is not a unique entity. There exist various possible unit cells.

A primitive cell is the smallest unit cell that can be repeated to form the lattice.

In many cases, it is more convenient to use a unit cell that is not a primitive cell.
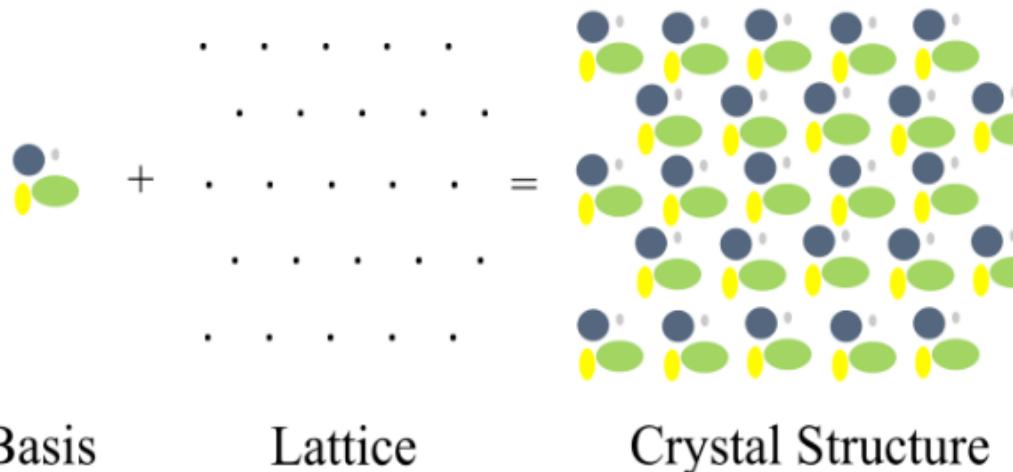
Unit cells may be chosen to have orthogonal sides.

Concepts of Crystal Structure: Basis and Lattice

Lattice + Basis=Crystal structure

Basis   Lattice   Crystal Structure
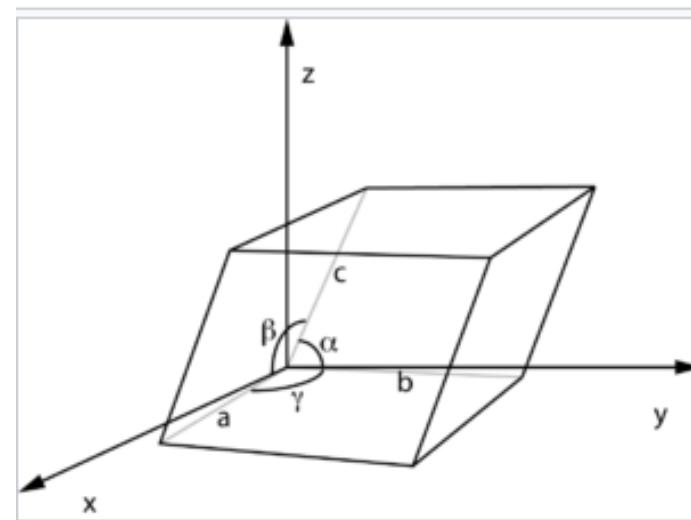
- Mathematical point of view, lattice is actually specific coordinates in space. The reason why these atoms are arranged regularly is because of they sit on the lattice.

# Concepts of Crystal Structure: Lattice Parameters
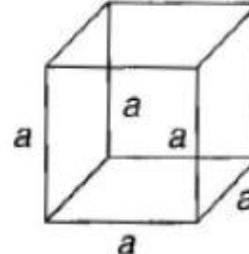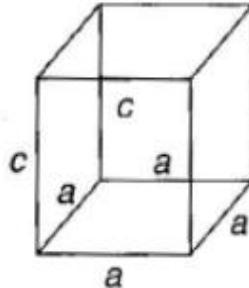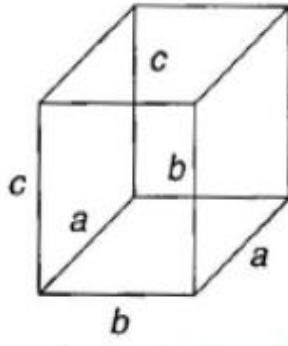
- **lattice constant**, or **lattice parameter**, refers to the physical dimension of unit cells in a crystal lattice.

- full set of lattice parameters consist of the three lattice constants (a,b,c) and the three angles (α, β,γ) between them.
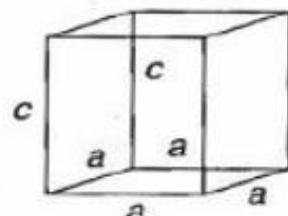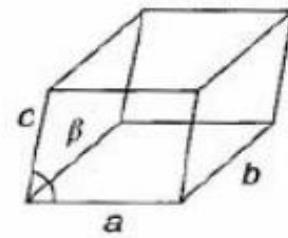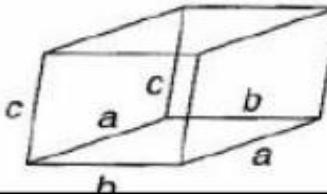
Crystal Systems

| System	Lattice constants and angles	Unit cell geometry
Cubic	$a = b = c,\ \alpha = \beta = \gamma = 90°$	
Tetragonal	$a = b \neq c,\ \alpha = \beta = \gamma = 90°$	
Orthorhombic	$a \neq b \neq c,\ \alpha = \beta = \gamma = 90°$	

| System	Axial lengths and angles	Unit cell geometry
Rhombohedral	$a = b = c,\ \alpha = \beta = \gamma \neq 90°$	
Hexagonal	$a = b \neq c,\ \alpha = \beta = 90°,\ \gamma = 120°$	
Monoclinic	$a \neq b \neq c,\ \alpha = \gamma = 90°,\ \neq \beta$	
Triclinic	$a \neq b \neq c,\ \alpha \neq \beta \neq \gamma \neq 90°$	
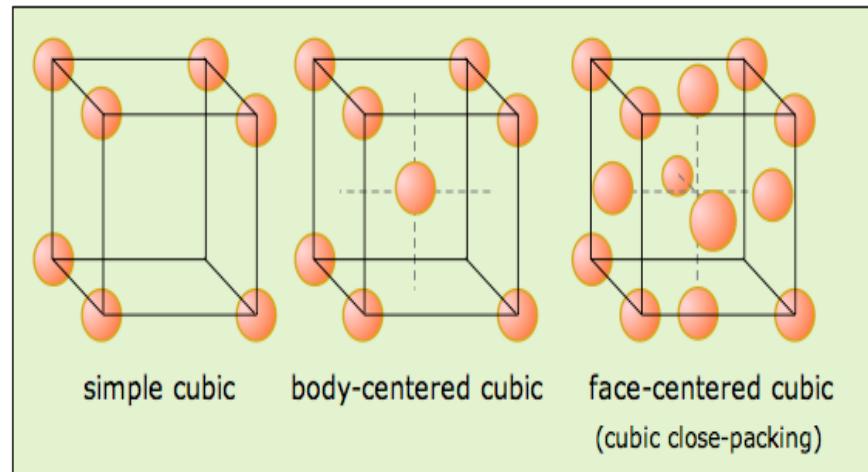
Unit cells

- Primitive unit cell:
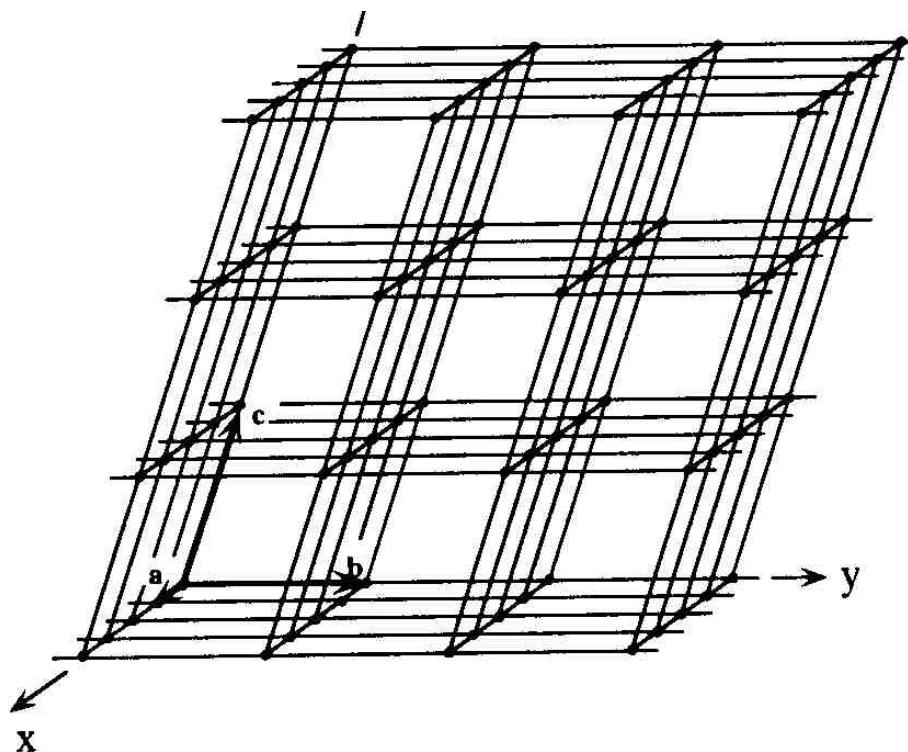
  When atoms in unit cell are present only at the corners

- Centered Unit Cells:

  When atoms are present at other positions in addition to corners in a unit cell

simple cubic   body-centered cubic   face-centered cubic
(cubic close-packing)
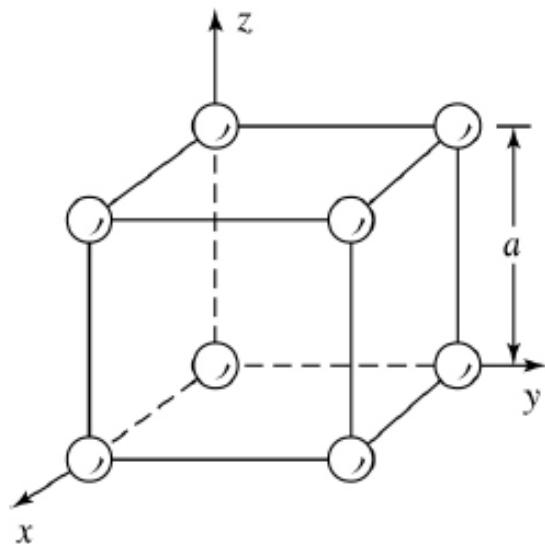
# A crystal lattice is a 3-D stack of unit cells
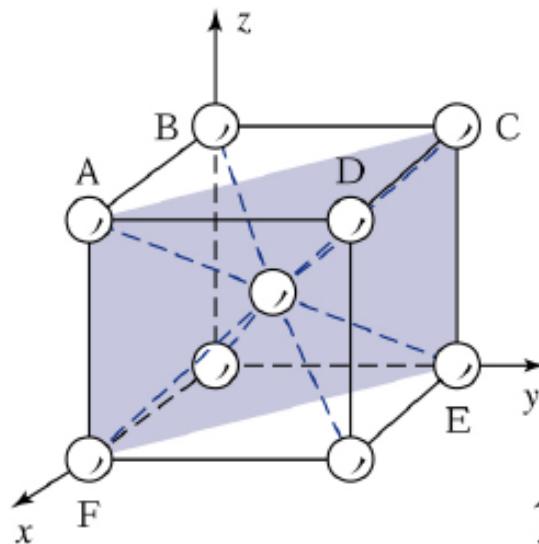
Crystal lattice is an imaginative grid system in three dimensions in which every point (or node) has an environment that is identical to that of any other point or node.
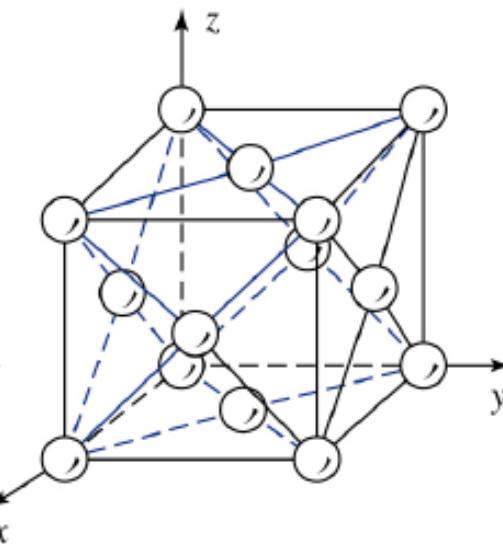
Examples of Some Basic Crystal Structures

(a) Simple cubic.　　　(b) Body-centered cubic.　　(c) Face-centered cubic.

For these structures, we can choose three vectors **a**, **b**, and **c** that are perpendicular to each other and equal in length.

The sc structure has an atom located at each corner. The bcc structure has additional atom at the center of the cube. The fcc structure has additional atoms on each face plane.

# Crystallographic Directions and Planes

- Crystal planes are defined as some imaginary planes inside a crystal in which large concentration of atoms are present. Inside the crystal, there exists certain directions along which large concentration of atoms exists. These directions are called crystal directions.

- Indices of crystallographic points, directions, and planes are given in terms of the lattice constants of the unit cell. For points and directions, you can consider the indices to be coefficients of the lattice constants. Remember that you only need to invert the indices for planes
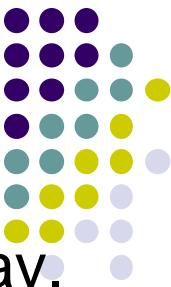
Bracket Conventions

- In crystallography there are conventions as to how the indices of planes and directions are written. When referring to a specific plane, "round" brackets are used:

- (*hkl*)

- When referring to a set of planes related by symmetry, then "curly" brackets are used:

- {*hkl*}

- These might be the (100) type planes in a cubic system, which are (100), (010), (001), (100),(010) and (001) . These planes all "look" the same and are related to each other by the symmetry elements present in a cube, hence their different indices depend only on the way the unit cell axes are defined. That is why it useful to consider the equivalent (010) set of planes.
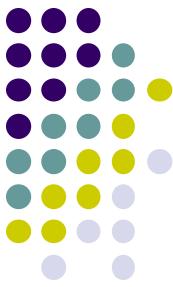
Bracket Conventions

- Directions in the crystal can be labeled in a similar way. These are effectively vectors written in terms of multiples of the lattice vectors **a**, **b**, and **c**. They are written with "square" brackets:

- [*UVW*]

- A number of crystallographic directions can also be symmetrically equivalent, in which case a set of directions are written with "triangular" brackets:

- *<UVW>*

Miller indices

A Miller index is a series of co-prime 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.
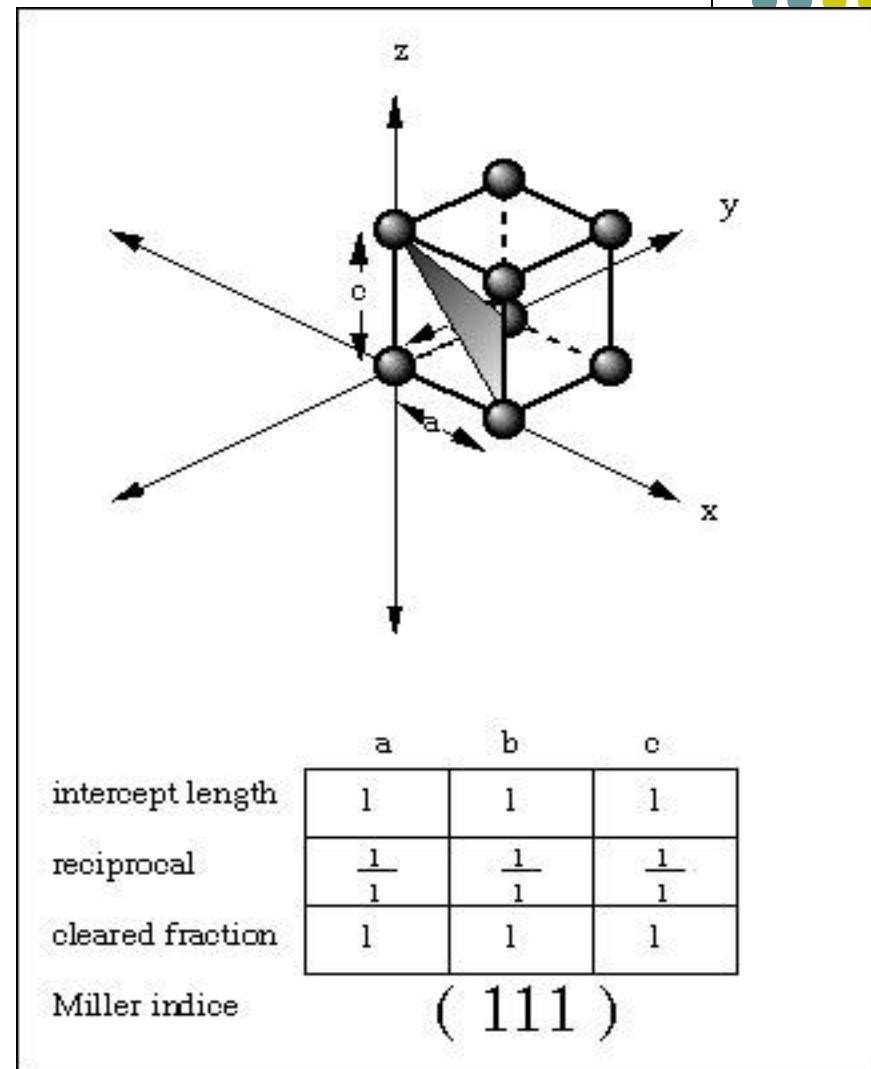
Miller Indices

Rules for determining Miller Indices:

1. Determine the intercepts of the face along the crystallographic axes, *in terms of unit cell dimensions.*
2. Take the reciprocals
3. Clear fractions
4. Reduce to lowest terms

An example of the (111) plane (h=1, k=1, l=1) is shown on the right.

|	a	b	c
intercept length	1	1	1
reciprocal	$\frac{1}{1}$	$\frac{1}{1}$	$\frac{1}{1}$
cleared fraction	1	1	1
Miller indice	(111)		
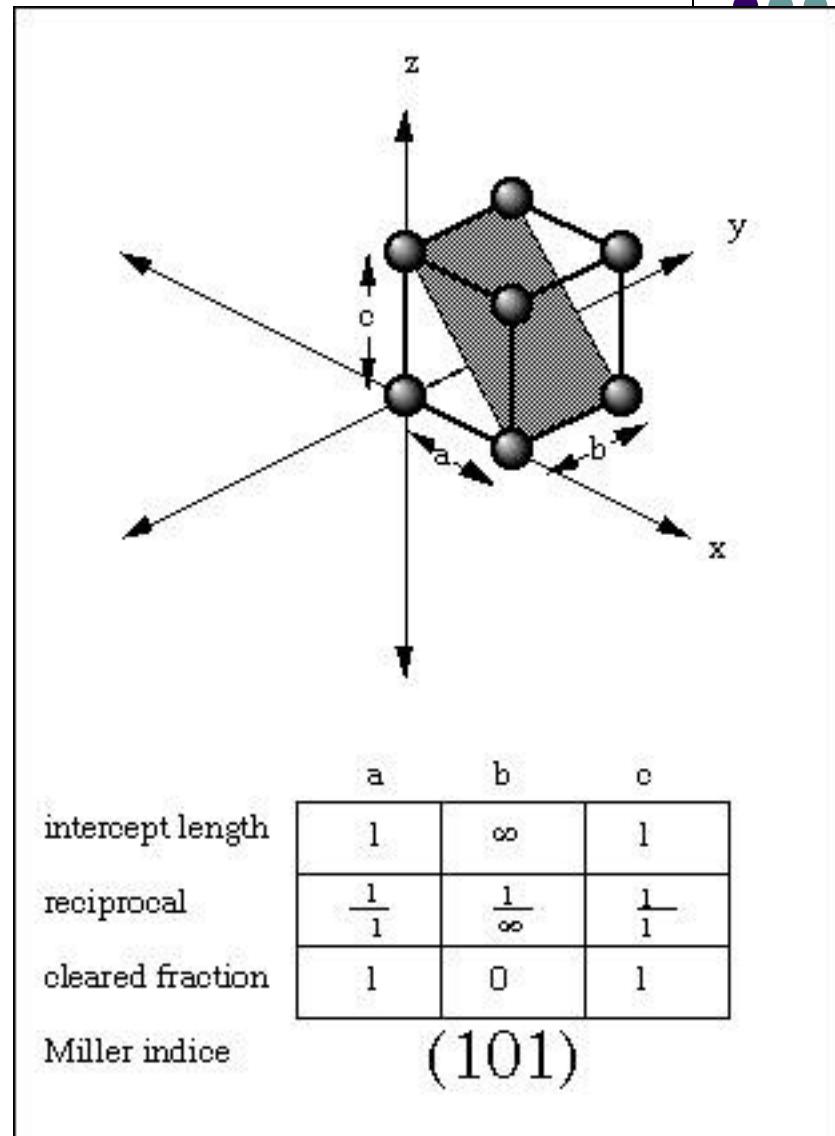
Another example:

Rules for determining Miller Indices:
1. Determine the intercepts of the face along the crystallographic axes, *in terms of unit cell dimensions.*
2. Take the reciprocals
3. Clear fractions
4. Reduce to lowest terms

	a	b	c
intercept length	1	∞	1
reciprocal	$\frac{1}{1}$	$\frac{1}{\infty}$	$\frac{1}{1}$
cleared fraction	1	0	1
Miller indice	(101)		
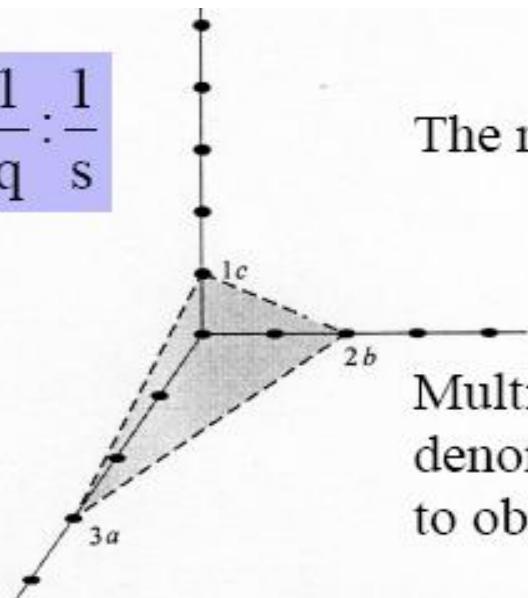
Crystal Planes and Miller Indices

Real crystals are not infinitely large. They have surfaces. Crystal surfaces are often related to different lattice planes. Lattice planes are characterized with **Miller indices (hkl)**, which are a set of integers with no common factors, inversely proportional to the intercepts of the crystal plane along the crystal axes:

$$h : k : 1 = \frac{1}{p} : \frac{1}{q} : \frac{1}{s}$$

$p = 3, q = 2, s = 1$

The reciprocals of the intercepts are

$$\left(\frac{1}{3}, \frac{1}{2}, \frac{1}{1} \right)$$

Multiply the smallest common denominator, which is 6 in this case, to obtain

$(hkl) = (2,3,6)$

Parallel lattice planes have same Miller indices and are entirely equivalent to each other.

Where does a protein crystallographer see the Miller indices?

- Common crystal faces are parallel to lattice planes

- Each diffraction spot can be regarded as a X-ray beam reflected from a lattice plane, and therefore has a unique Miller index.
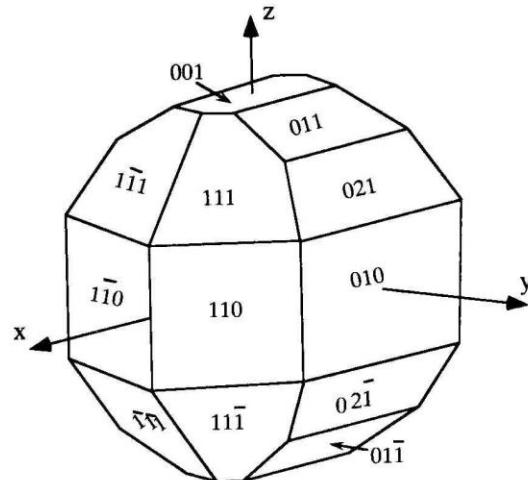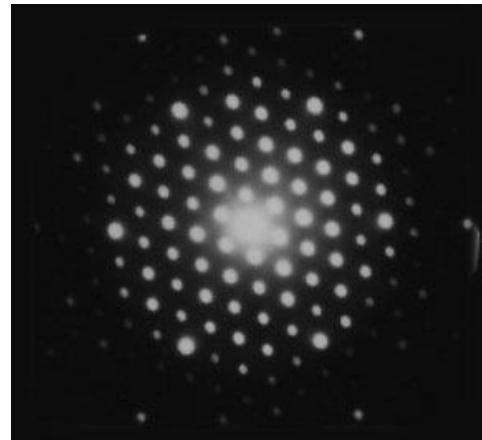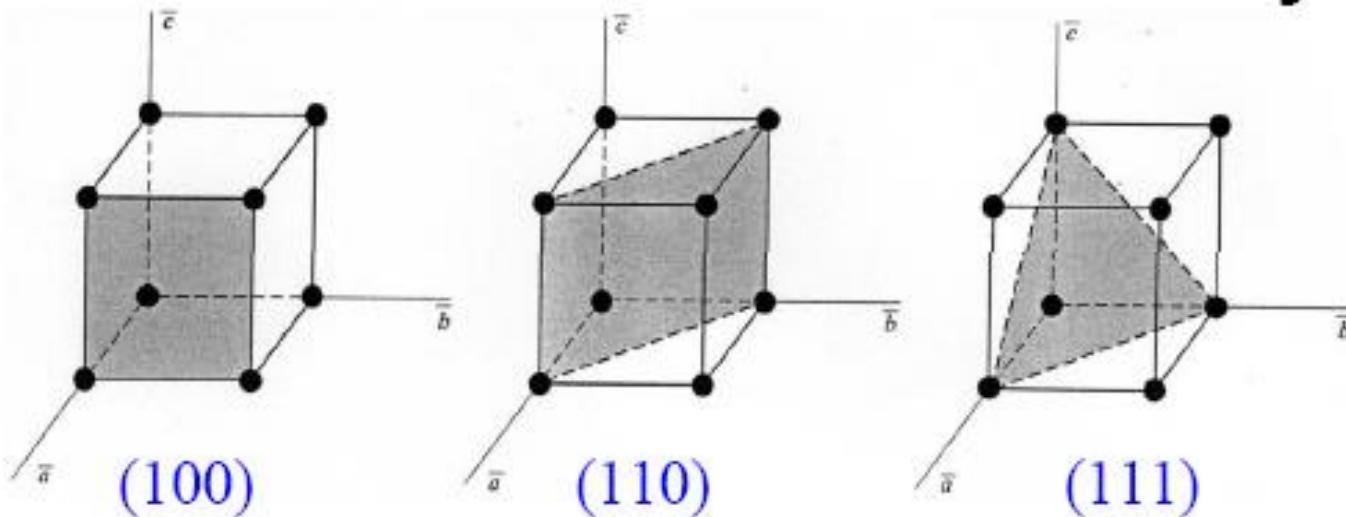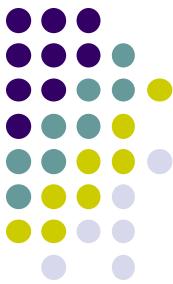
Figure 3.7. A crystal showing several faces.
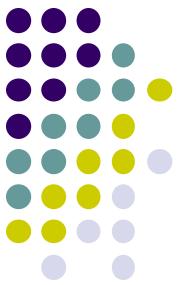
Common Lattice Planes in Cubic Crystals

(100)   (110)   (111)

1. When planes are parallel to certain axes, the corresponding intercepts will be ∞ and thus the reciprocals will be zeros.
2. If a plane passes through the origin, we would obtain infinity as one or more of the Miller indices. However, we can avoid the use of infinity by translating the origin to another equivalent lattice point since the location of the origin is entirely arbitrary.
3. Each face plane of the sc structure is entirely equivalent. These planes are grouped together and referred to as the **{100}** set of planes.
4. The distance between parallel lattice planes and the concentrations of atoms in specific planes are important parameters.
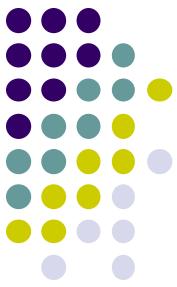
Symmetry

A state in which parts on opposite sides of a plane, line, or point display arrangements that are related to one another via a symmetry operation such as
translation, rotation, reflection or inversion.

Application of the symmetry operators leaves the entire crystal unchanged.

Symmetry Elements:
Translation

uT

The first point is repeated at equal distances along a line by a translation uT, where T is the translation vector and u is an integer
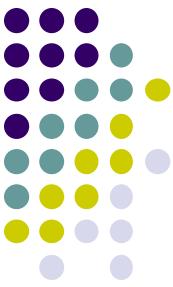
Symmetry Elements:
Translation
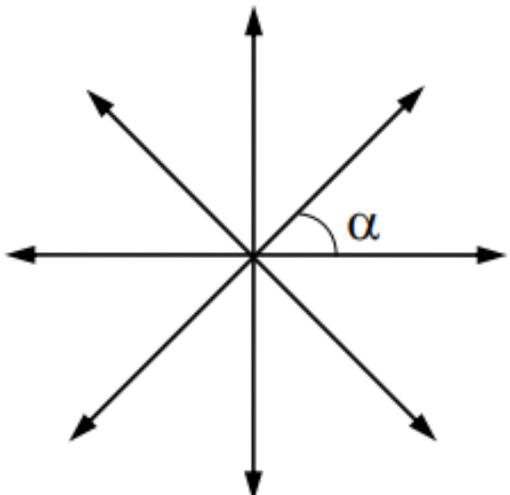
moves all the points in the asymmetric unit the same distance in the same direction. This has no effect on the handedness of figures in the plane. There are no invariant points (points that map onto themselves) under a translation.
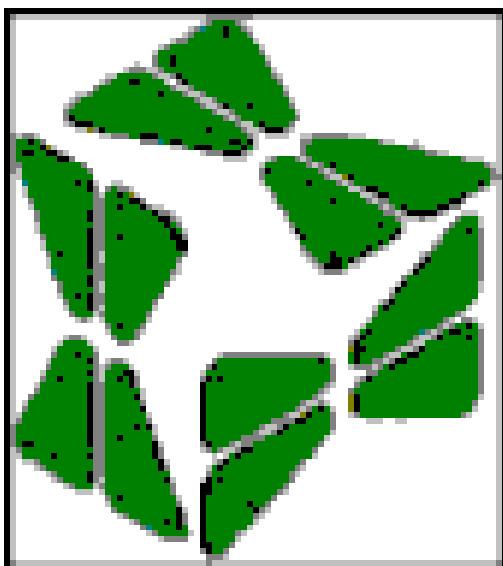
Symmetry Elements:
Rotation

A rotation can be applied on the translation vector T in all directions, clock or anti-clock wise, through equal angles α, Because of the regular pattern, the translation between these two points will be some multiple of T (pT)

Symmetry Elements:
Rotation

turns all the points in the asymmetric unit around one axis, the center of rotation. A rotation does not change the handedness of figures. The center of rotation is the only invariant point (point that maps onto itself).

Symmetry Elements:
Rotation
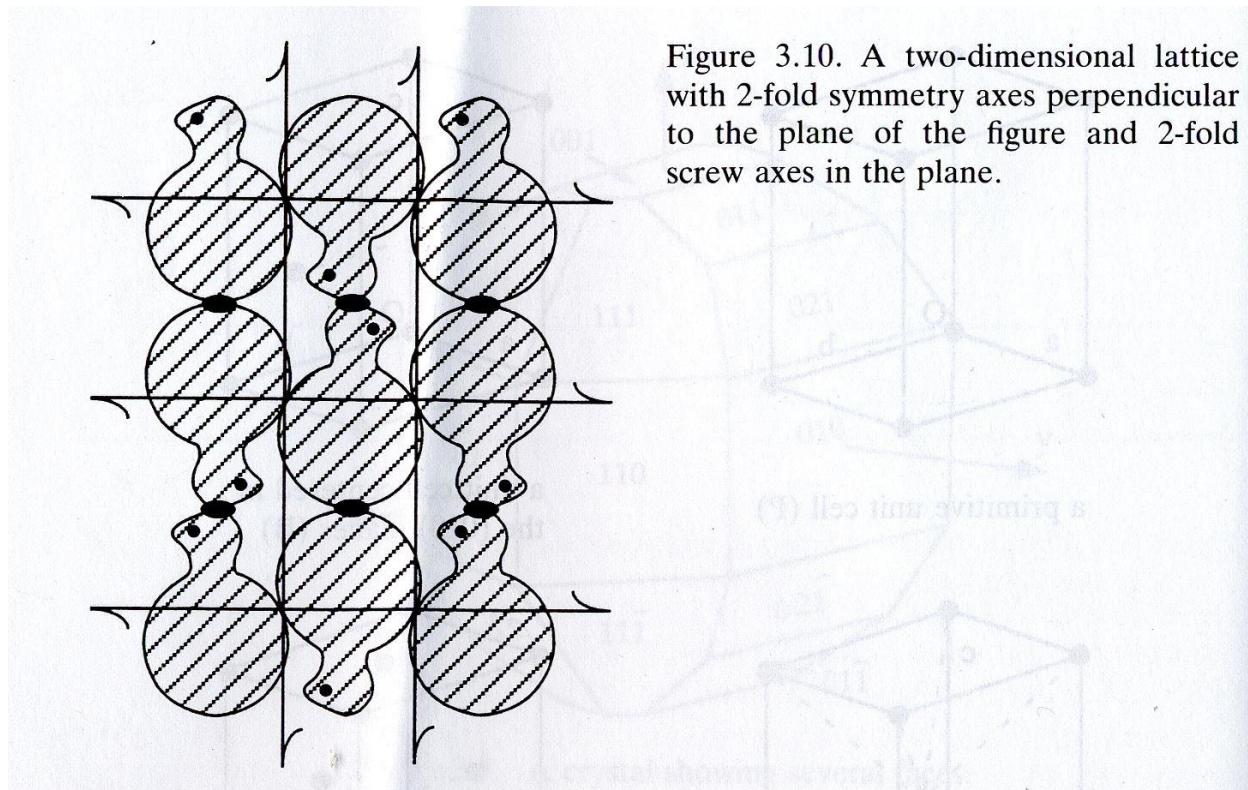
Figure 3.10. A two-dimensional lattice with 2-fold symmetry axes perpendicular to the plane of the figure and 2-fold screw axes in the plane.

Symmetry Elements:
Rotation
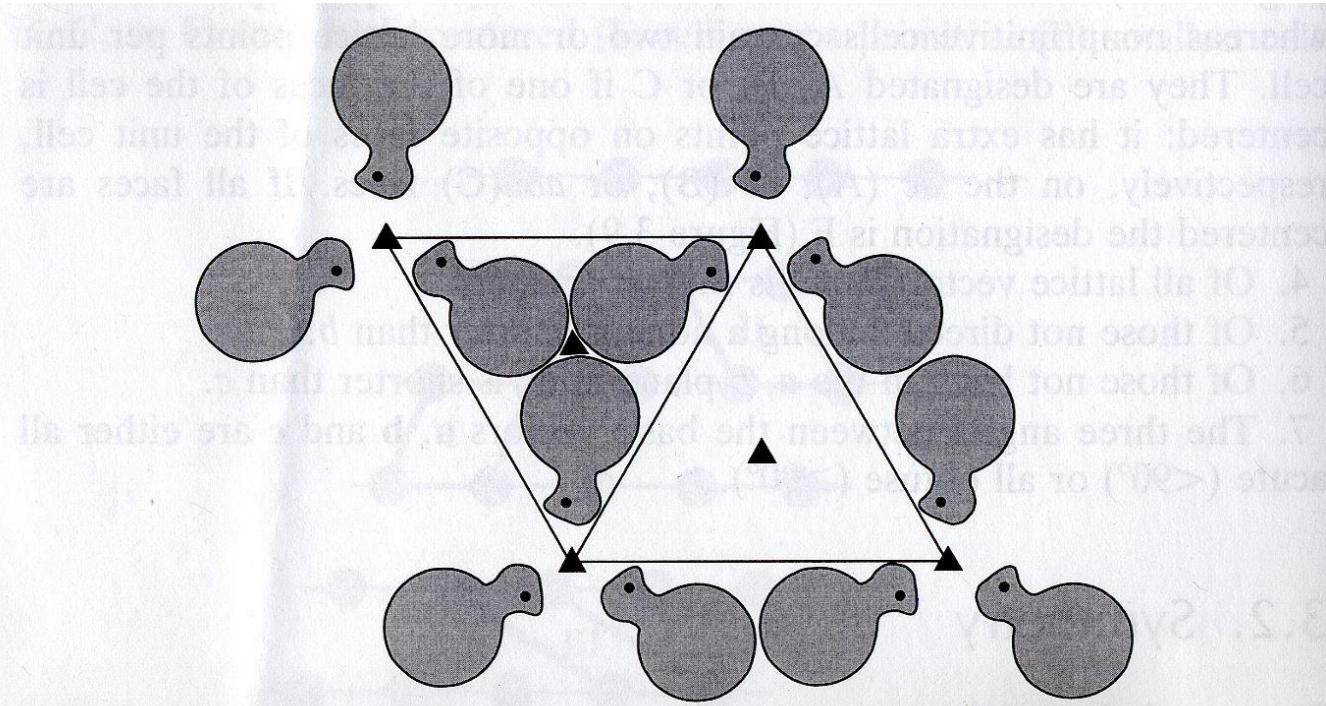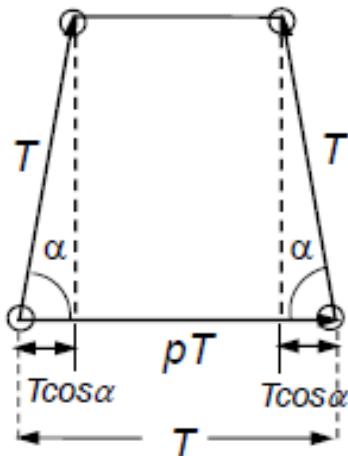
Figure 3.11. A two-dimensional lattice with 3-fold symmetry axes perpendicular to the plane of the figure.

Symmetry operations

Rotation

$$T = T \cos\alpha + pT + T \cos\alpha = pT + 2T \cos\alpha$$

$$\cos \alpha = (1 - p)/2$$
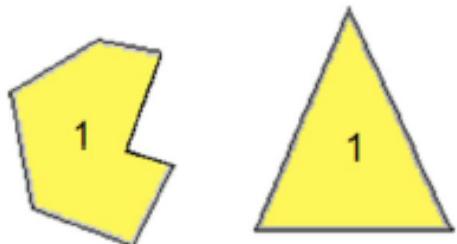
p	α°	n-fold	Symbol
0	60	6	⬡
1	90	4	■
2	120	3	▲
3	180	2	⬗
-1	0/360	1	

An n-fold rotation symmetry means rotation through an angle of $2\pi/n$ will repeat the object or motif n times in a full $360°$ rotation. n =1 means no symmetry.
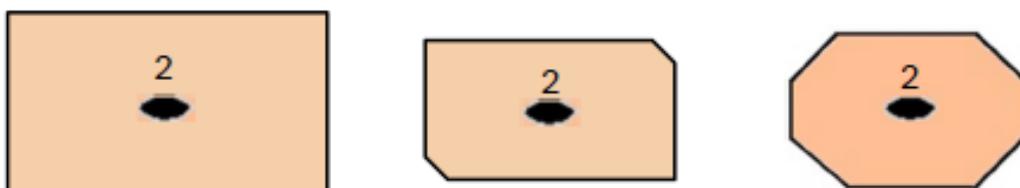
Rotation

1-Fold Rotation Axis - An object that requires rotation of a full 360° to repeat itself has no rotational symmetry.
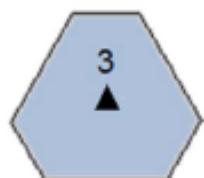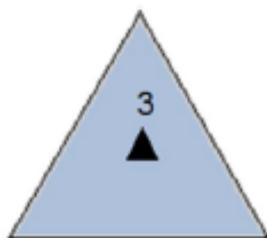
2-fold Rotation Axis - If an object appears identical after a rotation of 180°, that is twice in a 360° rotation, then it is said to have a 2-fold (2π/180) rotation symmetry
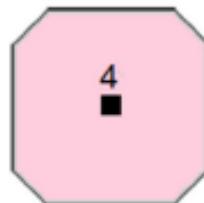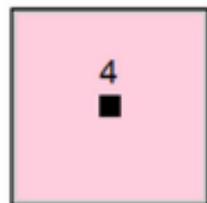
Rotation
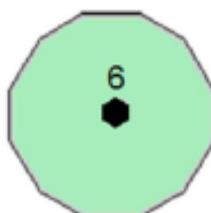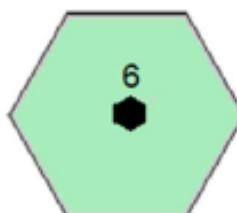
Similarly we have 3, 4 and 6-fold rotational symmetry

3 fold – $2\pi/120$

4 fold – $2\pi/90$

6 fold – $2\pi/60$
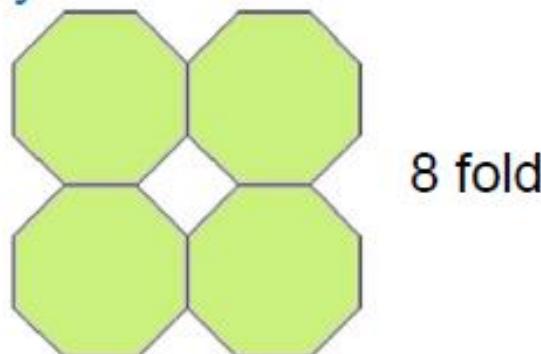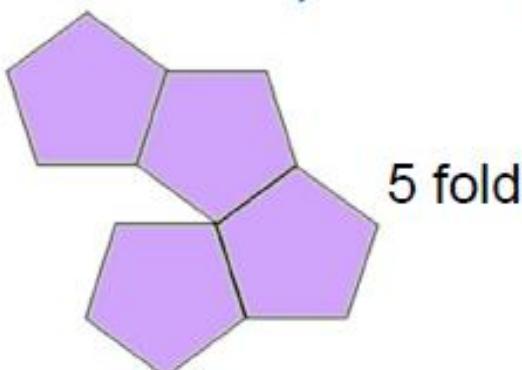
Rotation

Is it possible to have 5, 7 or 8-fold rotation symmetry?

Objects with 5, 7 and 8 or higher order symmetry do exist in nature, e.g. star fish (5-fold), flowers with 5 or 8-fold symmetry.
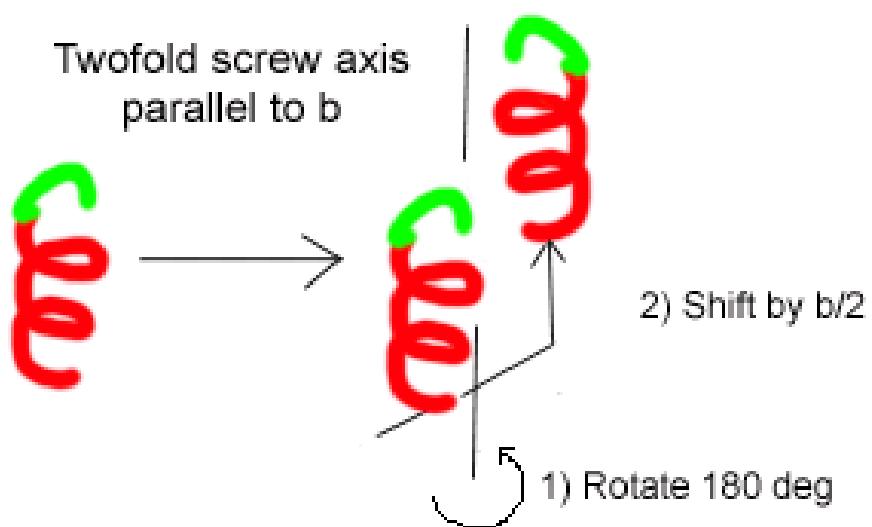
However, these are not possible in crystallography as they cannot fill the space completely

5 fold

8 fold

Symmetry Elements
Screw axes (rotation + translation)

Twofold screw axis parallel to b

1) Rotate 180 deg

2) Shift by b/2

rotation about the axis of symmetry by 360°/n, followed by a translation parallel to the axis by r/n of the unit cell length in that direction. (r < n)

Symmetry Elements
Screw axes (rotation + translation)

120° rotation
1/3 unit cell translation
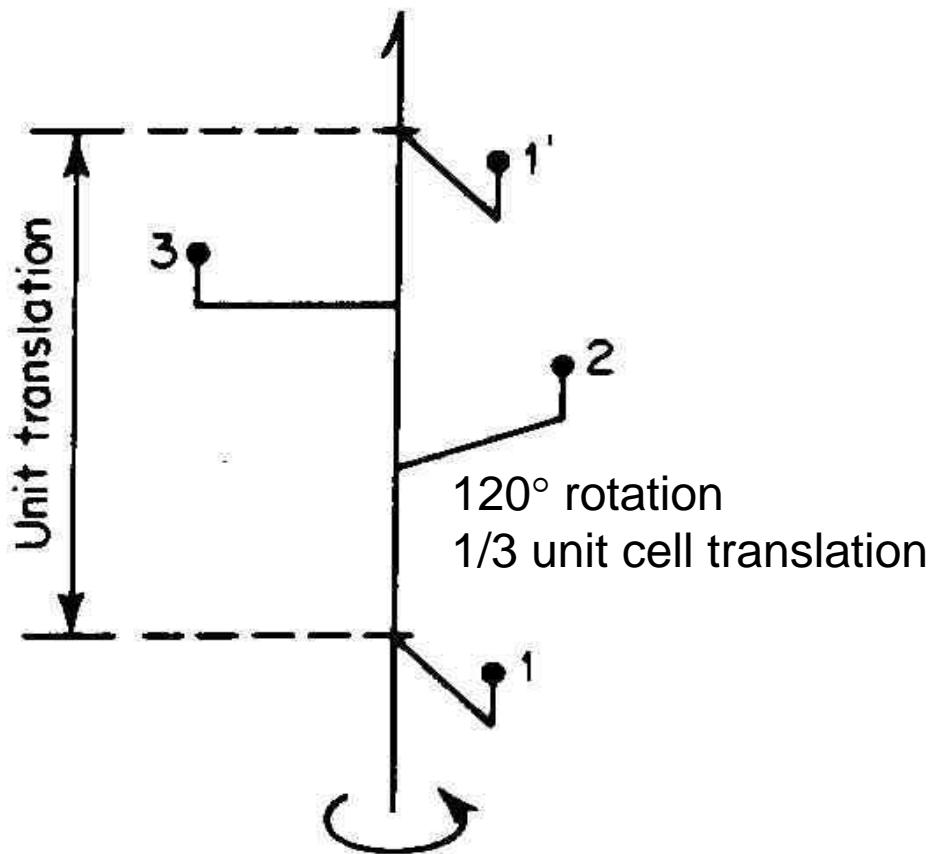
Figure 3.20. Screw axis 3_1.
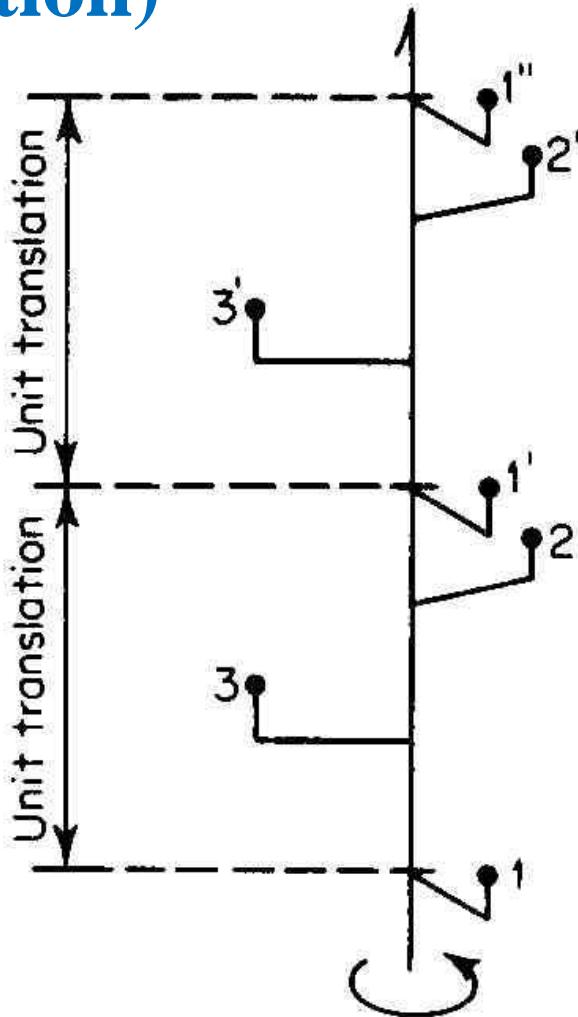
Figure 3.21. Screw axis 3_2.
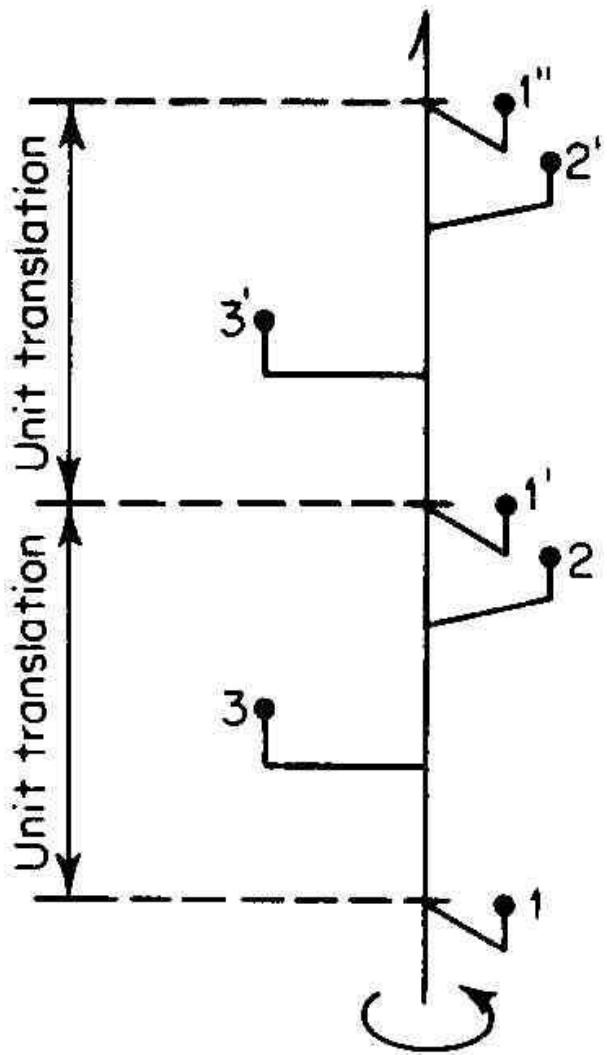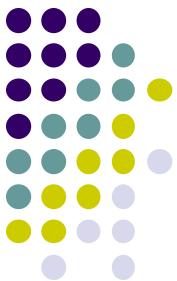
Figure 3.21. Screw axis 3_2.
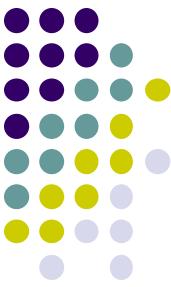
Symmetry Elements
Inversion, or center of symmetry

x, y, z

$\bar{x}, \bar{y}, \bar{z}$
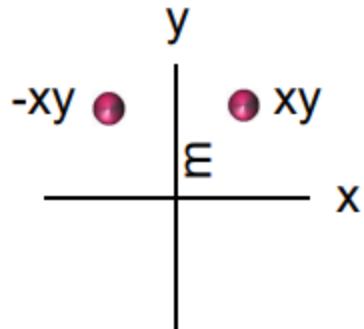
every point on one side of a center of symmetry has a similar point at an equal distance on the opposite side of the center of symmetry.

Symmetry Elements
Reflection or Mirror symmetry
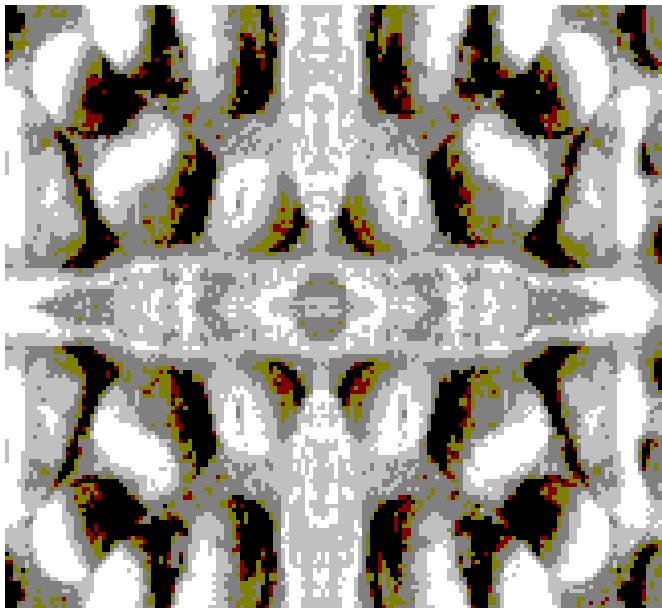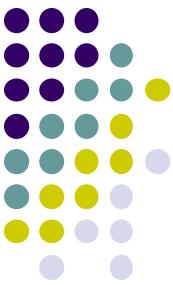
An object with a reflection symmetry will be a mirror image of itself across a plane called mirror plane (m).
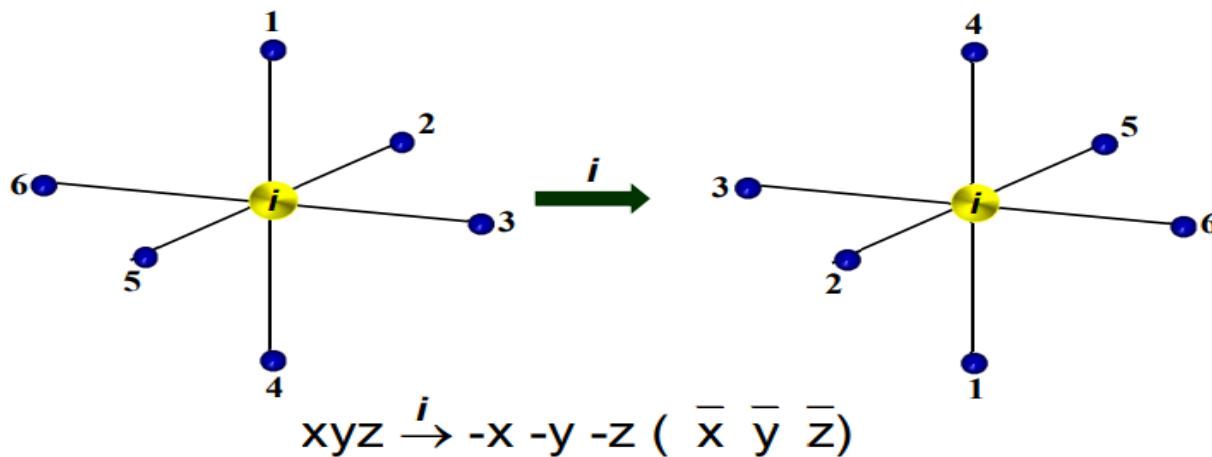
Symmetry Elements
## Reflection or Mirror symmetry

flips all points in the asymmetric unit over a line, which is called the mirror, and thereby changes the handedness of any figures in the asymmetric unit.
The points along the mirror line are all invariant points (points that map onto themselves) under a reflection.
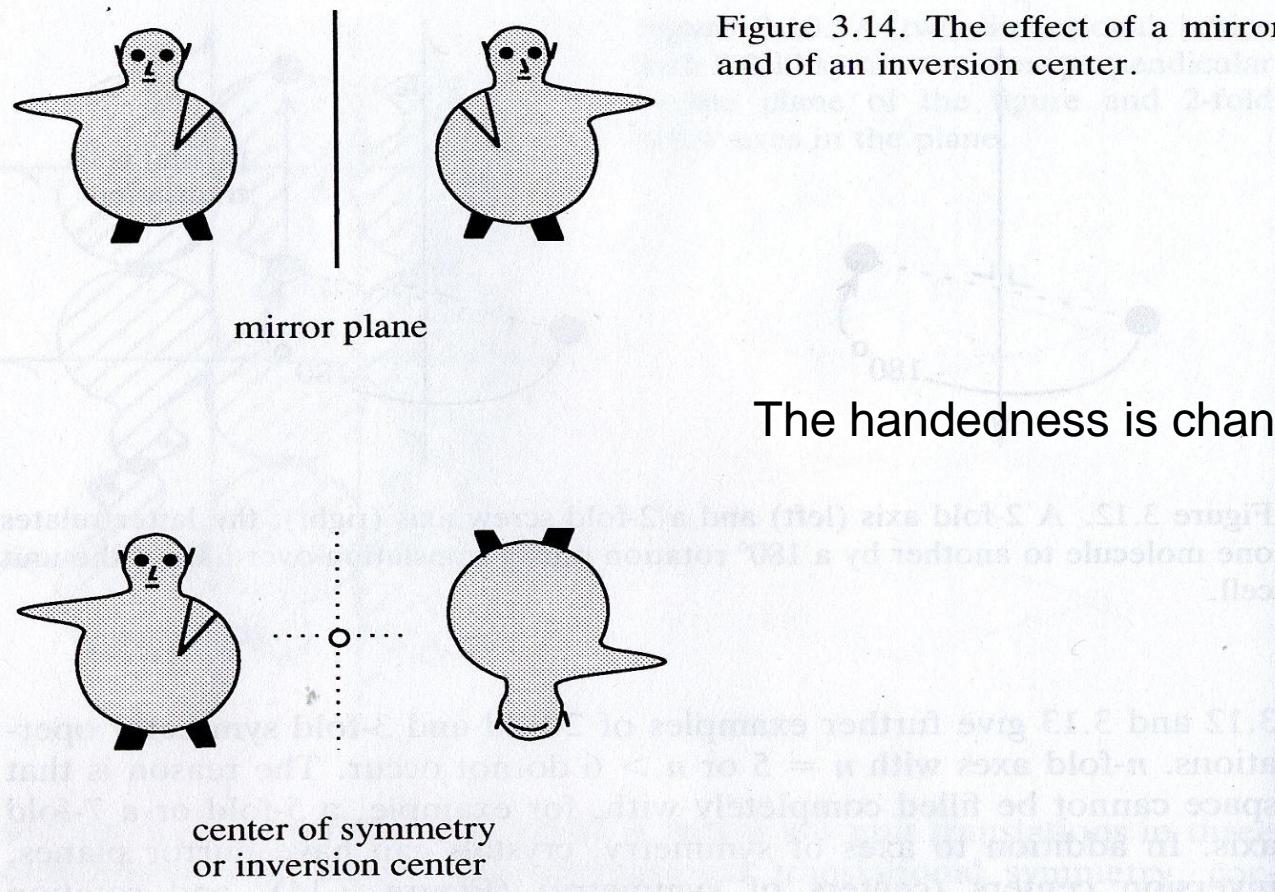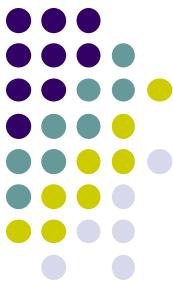
Symmetry Elements
Inversion symmetry

$$xyz \xrightarrow{i} -x\ -y\ -z\ (\ \overline{x}\ \overline{y}\ \overline{z})$$

In this operation, every part of the object is reflected through an inversion center called center of symmetry which is denoted as i. The object is reproduced inverted from its original position.

# Symmetry elements: mirror plane and inversion center

Figure 3.14. The effect of a mirror and of an inversion center.

mirror plane

The handedness is changed.

center of symmetry or inversion center

Symmetry Elements
Glide reflection (mirror plane + translation)

axis of a glide
reflection

reflects the asymmetric unit across a mirror and then translates parallel to the mirror. A glide plane changes the handedness of figures in the asymmetric unit. There are no invariant points (points that map onto themselves) under a glide reflection.
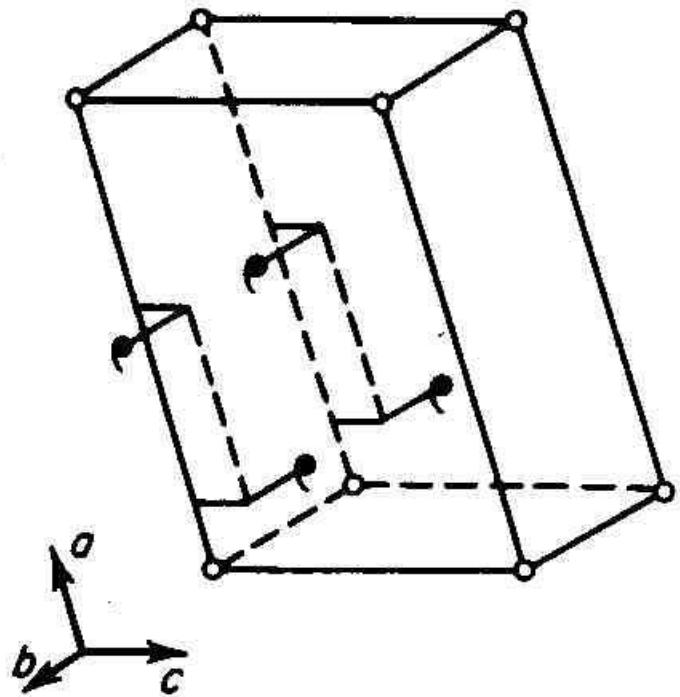
Figure 3.22. Glide plane *a*.

Table 3.1. Graphic Symbols for Symmetry Elements[a]

Symmetry axis or symmetry point	Graphic symbol	Screw vector of a right-handed screw rotation in units of the shortest lattice translation vector parallel to the axis	Printed symbol
Symmetry axes normal to the plane of projection (three dimensions) and symmetry points in the plane of the figure (two dimensions)			
Identity	None	None	1
Twofold rotation axis Twofold rotation point (two dimensions)	◗	None	2
Twofold screw axis: "2 sub 1"	◗	$\frac{1}{2}$	2_1
Threefold rotation axis Threefold rotation point (two dimensions)	▲	None	3
Threefold screw axis: "3 sub 1"	▲	$\frac{1}{3}$	3_1
Three fold screw axis: "3 sub 2"	▲	$\frac{2}{3}$	3_2
Fourfold rotation axis Fourfold rotation point (two dimensions)	◆	None	4
Fourfold screw axis: "4 sub 1"	◆	$\frac{1}{4}$	4_1
Fourfold screw axis: "4 sub 2"	◆	$\frac{1}{2}$	4_2
Fourfold screw axis: "4 sub 3"	◆	$\frac{3}{4}$	4_3
Sixfold rotation axis Sixfold rotation point (two dimensions)	⬣	None	6

(continued)

Point and Space groups

Symmetry operations generate a variety of arrangements of lattice points in three dimensions. There are **32** unique ways in which lattice points can be arranged in space. These non-translation elements are called *point-groups*.

A large number of 3D structures are generated when translations [linear translation, translation + reflection (glide plane) and translation + rotation (screw axis)] are applied to the point groups. There are **230** unique shapes which can be generated this way. These are called *space groups*.
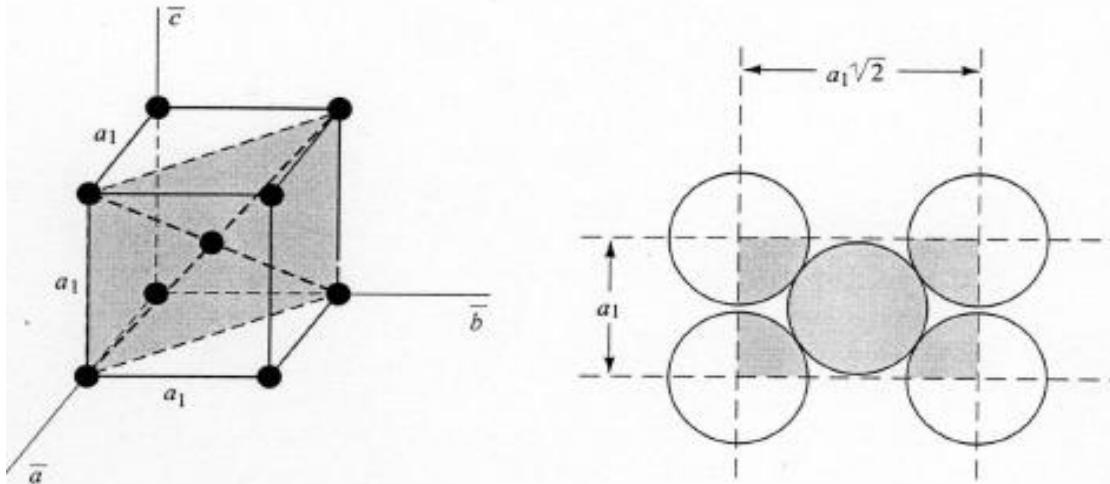
Surface Density of Atoms on a Particular Plane

Example: consider the bcc structure. Assume the atoms can be represented as hard
spheres with the closest atoms toughing each other and the lattice constant is 0.5 nm.
Calculate the surface density of atoms on the (110) plane.

Consider the atoms on the (110) plane. The atom at each corner is shared by
four similar rectangles. So one fourth of each atom at the corner contributes
to the shaded rectangle. The four corner atoms effectively contribute one
atom to the shaded rectangle. The atom at the center is not shared by any
other rectangle. It is entirely included in the shaded rectangle. Therefore, the
shaded rectangle contains two atoms.

Surface Density of Atoms on a Particular Plane

Solution: the surface density is found by dividing the number of lattice atoms by the surface area.

$$\text{Surface density } = \frac{2}{(a_1)(a_1\sqrt{2})} = \frac{2}{(5\times10^{-8})^2(\sqrt{2})} = 5.66\times10^{14} \text{ atoms per cm}^2$$

The surface density of atoms is a function of the particular crystal plane and generally varies from one crystal plane to another.

Description of directions in a lattice:
In addition to lattice planes, we also want to describe a particular direction in the crystal. The direction can be expressed as a set of three integers that are the components of a vector in that direction. For example, the body diagonal in the sc lattice has vector components of 1,1,1. The body diagonal is then described as the **[111]** direction. The brackets are used to designate direction as distinct from the parentheses used for crystal planes.
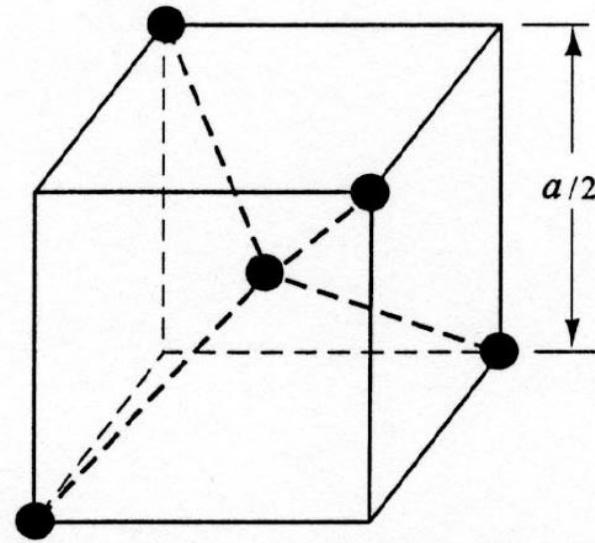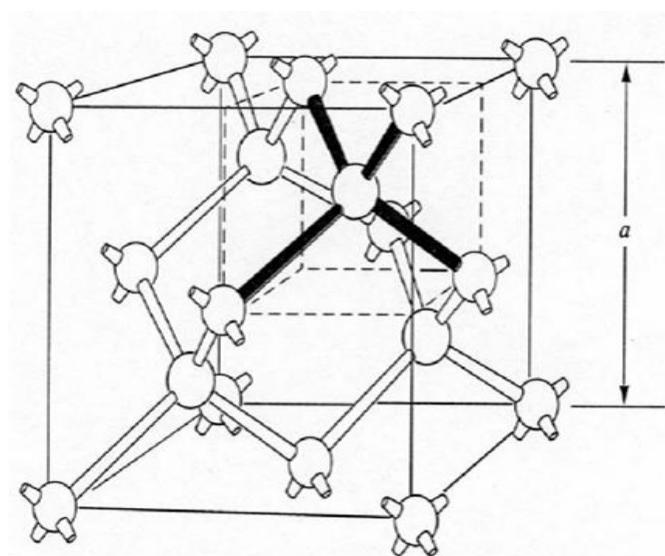
The Diamond Structure
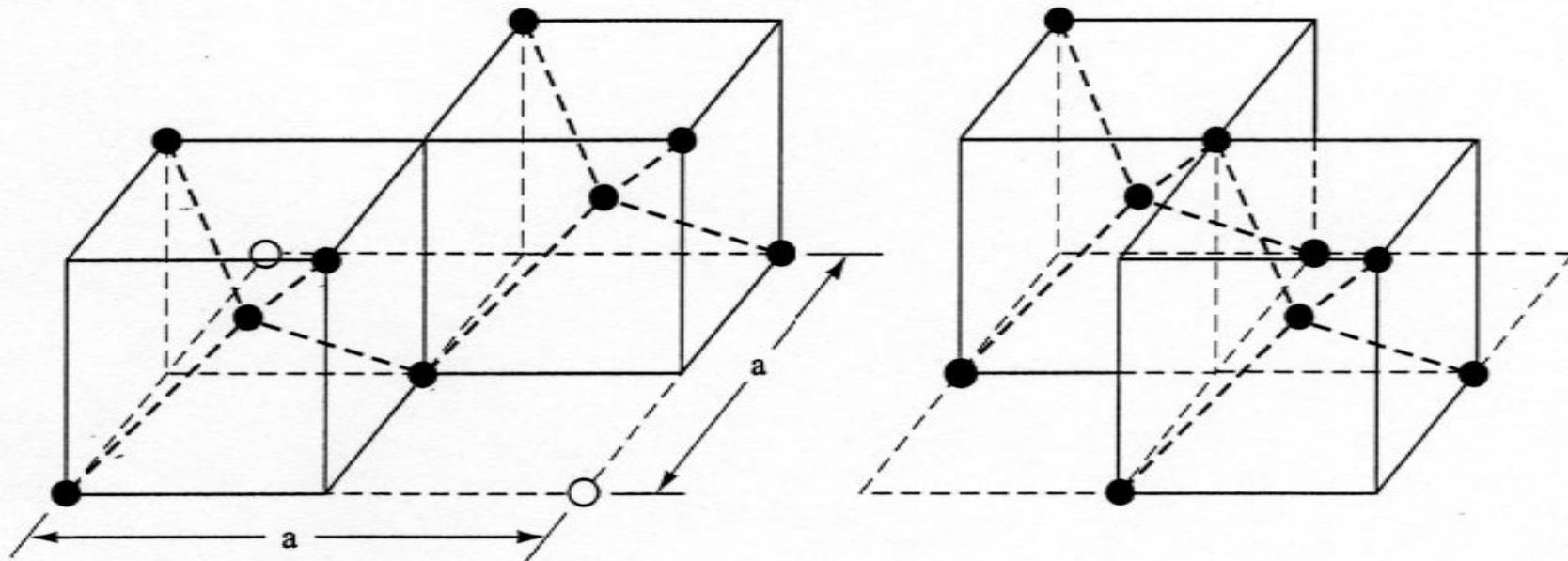
Silicon is the most common semiconductor material. Both silicon and germanium have a diamond crystal structure.

The basic building block of the diamond structure is the tetrahedral structure.

The Diamond Structure
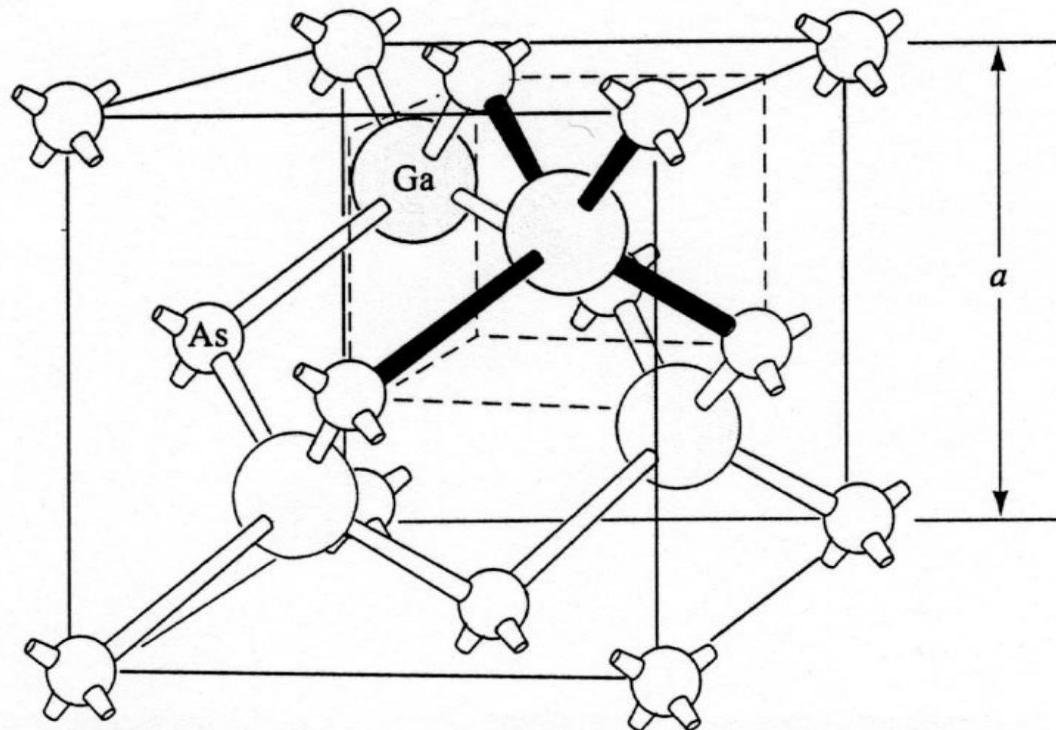
An important characteristic of the diamond structure is that any atom in the structure has four nearest neighboring atoms.

All atoms in the diamond structure are of the same species, such as silicon or germanium.

The Zincblende (Sphalerite) Structure

The zincblende (sphalerite) structure differs from the diamond structure only in that there are two different types of atoms in the structure.
Compound semiconductors, such as GaAs, have the zincblende structure.
The important feature of both the diamond and zincblende structure is that the atoms are joined together to form tetrahedrons.

Classification of lattice

The **Seven** Crystal System

And

The **Fourteen** Bravais Lattices

Auguste Bravais
(1811-1863)
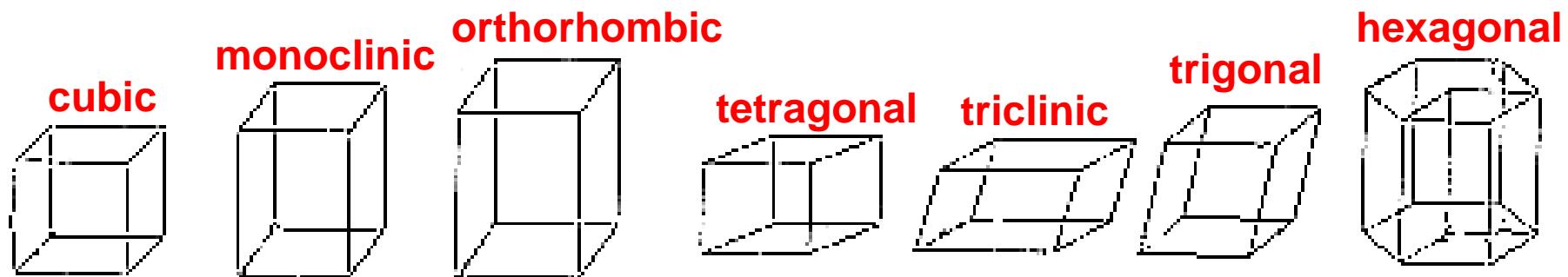
Lattices

- In 1848, Auguste Bravais demonstrated that in a 3-dimensional system there are fourteen possible lattices

- A Bravais lattice is an infinite array of discrete points with identical environment

- seven crystal systems + four lattice centering types = 14 Bravais lattices

- Lattices are characterized by translation symmetry

7 Crystal Systems

cubic monoclinic orthorhombic tetragonal triclinic trigonal hexagonal

Crystal System	External Minimum Symmetry	Unit Cell Properties
Triclinic	None	a, b, c, al, be, ga,
Monoclinic	One 2-fold axis, || to b (b unique)	a, b, c, 90, be, 90
Orthorhombic	Three perpendicular 2-folds	a, b, c, 90, 90, 90
Tetragonal	One 4-fold axis, parallel c	a, a, c, 90, 90, 90
Trigonal	One 3-fold axis	a, a, c, 90, 90, 120
Hexagonal	One 6-fold axis	a, a, c, 90, 90, 120
Cubic	Four 3-folds along space diagonal	a, a, ,a, 90, 90, 90
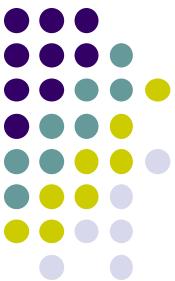
Four lattice centering types

| No.	Type	Description
1	Primitive	Lattice points on corners only. Symbol: P.
2	Face Centered	Lattice points on corners as well as centered on faces. Symbols: A (bc faces); B (ac faces); C (ab faces).
3	All-Face Centered	Lattice points on corners as well as in the centers of all faces. Symbol: F.
4	Body-Centered	Lattice points on corners as well as in the center of the unit cell body. Symbol: I.
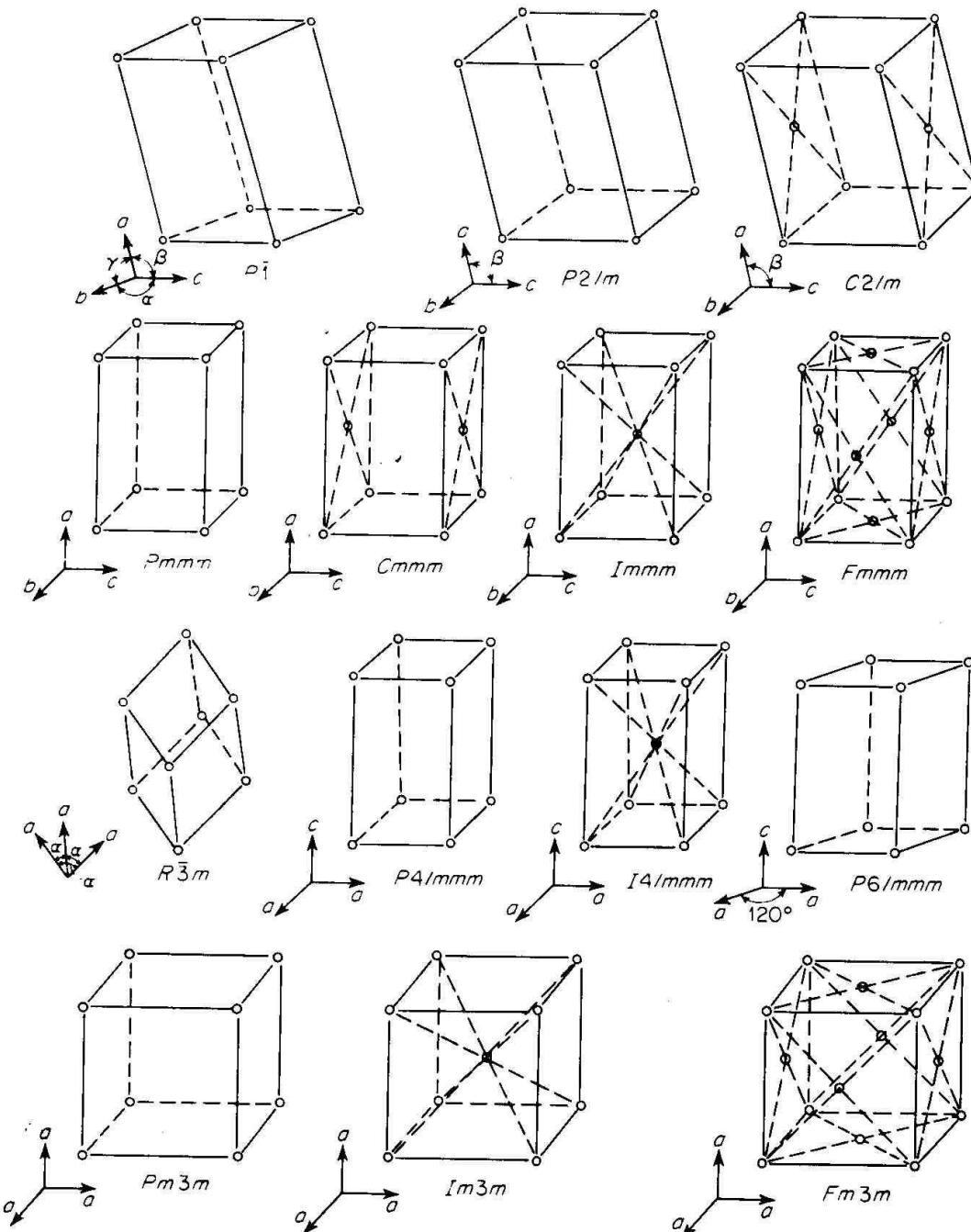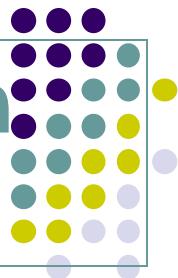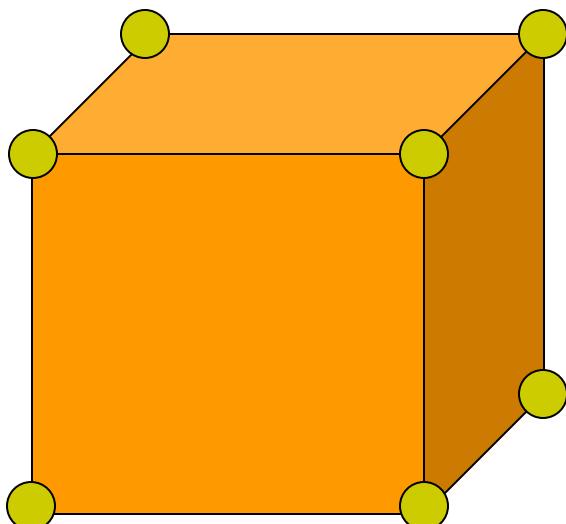
Figure 3.13. The 14 Bravais lattices.

Crystal Physics

14 Bravais lattices divided into seven crystal systems

Crystal system   ## Bravais lattices

1. Cubic   P   I   F

Simple cubic
Primitive cubic
Cubic P
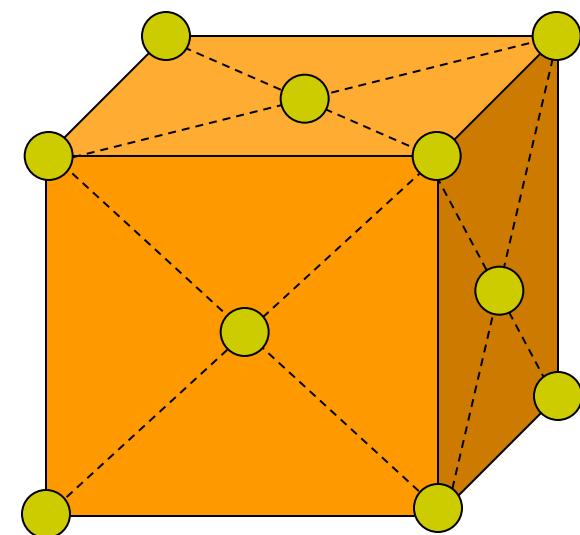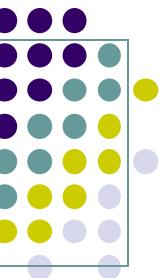
Body-centred cubic
Cubic I
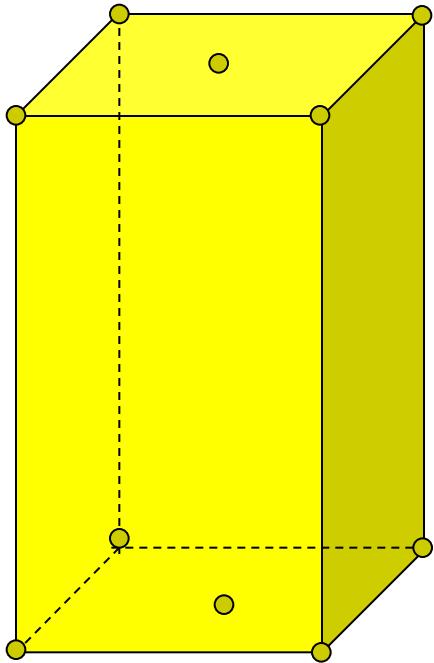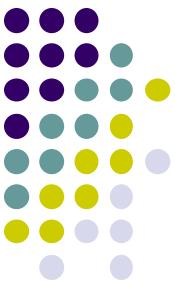
Face-centred cubic
Cubic F
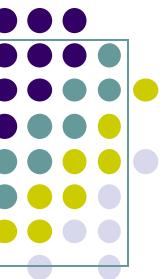
14 Bravais lattices divided into seven crystal systems

| Crystal system	Bravais lattices			
1. Cubic	P	I	F	
2. Tetragonal	P	I		
3. Orthorhombic	P	I	F	C
4. Hexagonal	P			
5. Trigonal	P			
6. Monoclinic	P			C
7. Triclinic	P			

Orthorhombic C
End-centred orthorhombic
Base-centred orthorhombic
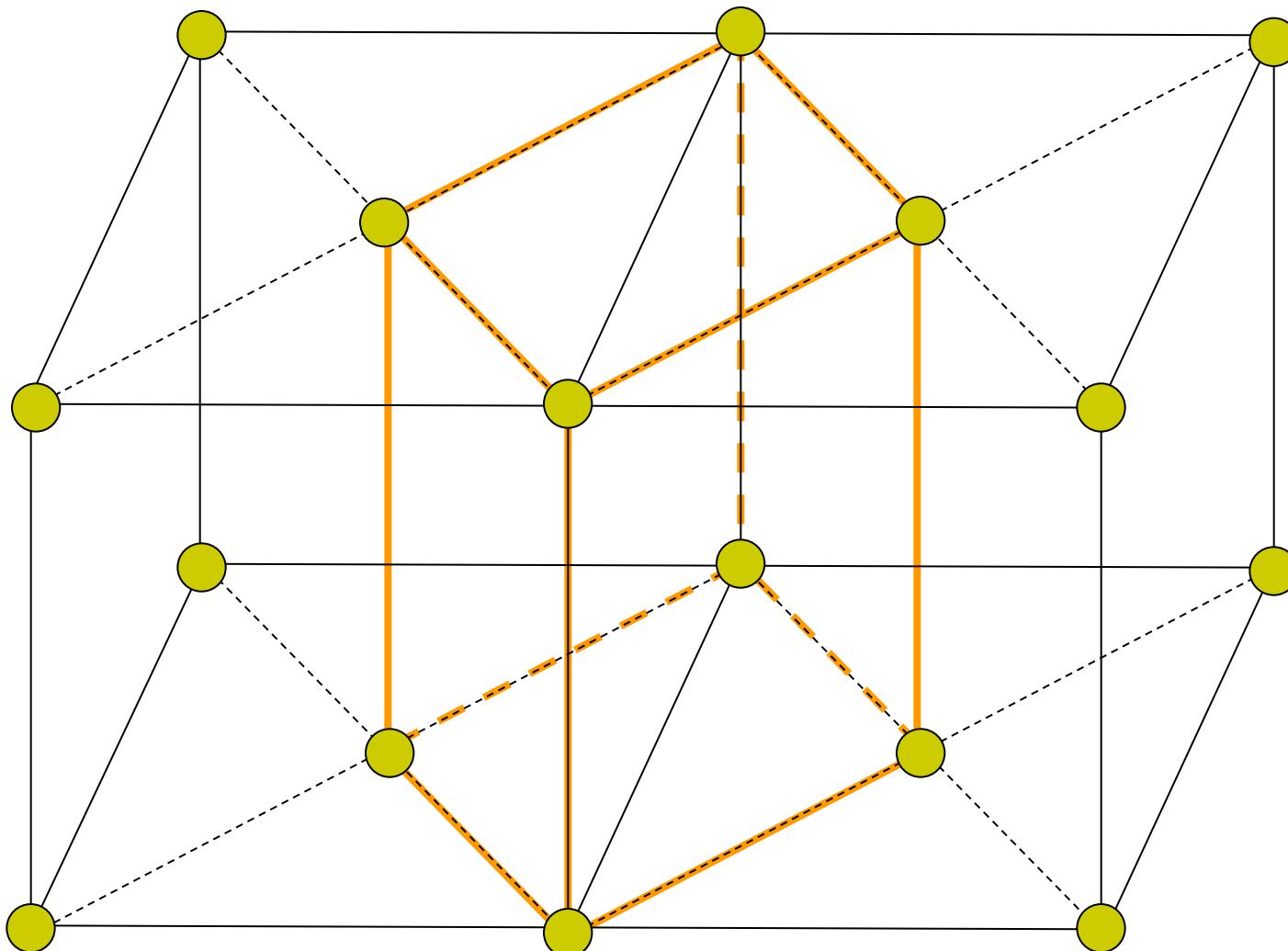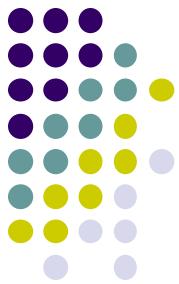
# 14 Bravais lattices divided into seven crystal systems

Crystal system   Bravais lattices

1. Cubic   P   I   F   ?

2. Tetragonal   P   I

3. Orthorhombic   P   I   F   C

4. Hexagonal   P

5. Trigonal   P

6. Monoclinic   P   C

7. Triclinic   P
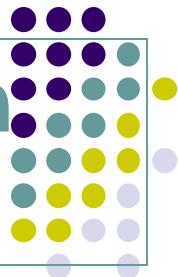
End-centred cubic not in the Bravais list ?

End-centred cubic = Simple Tetragonal
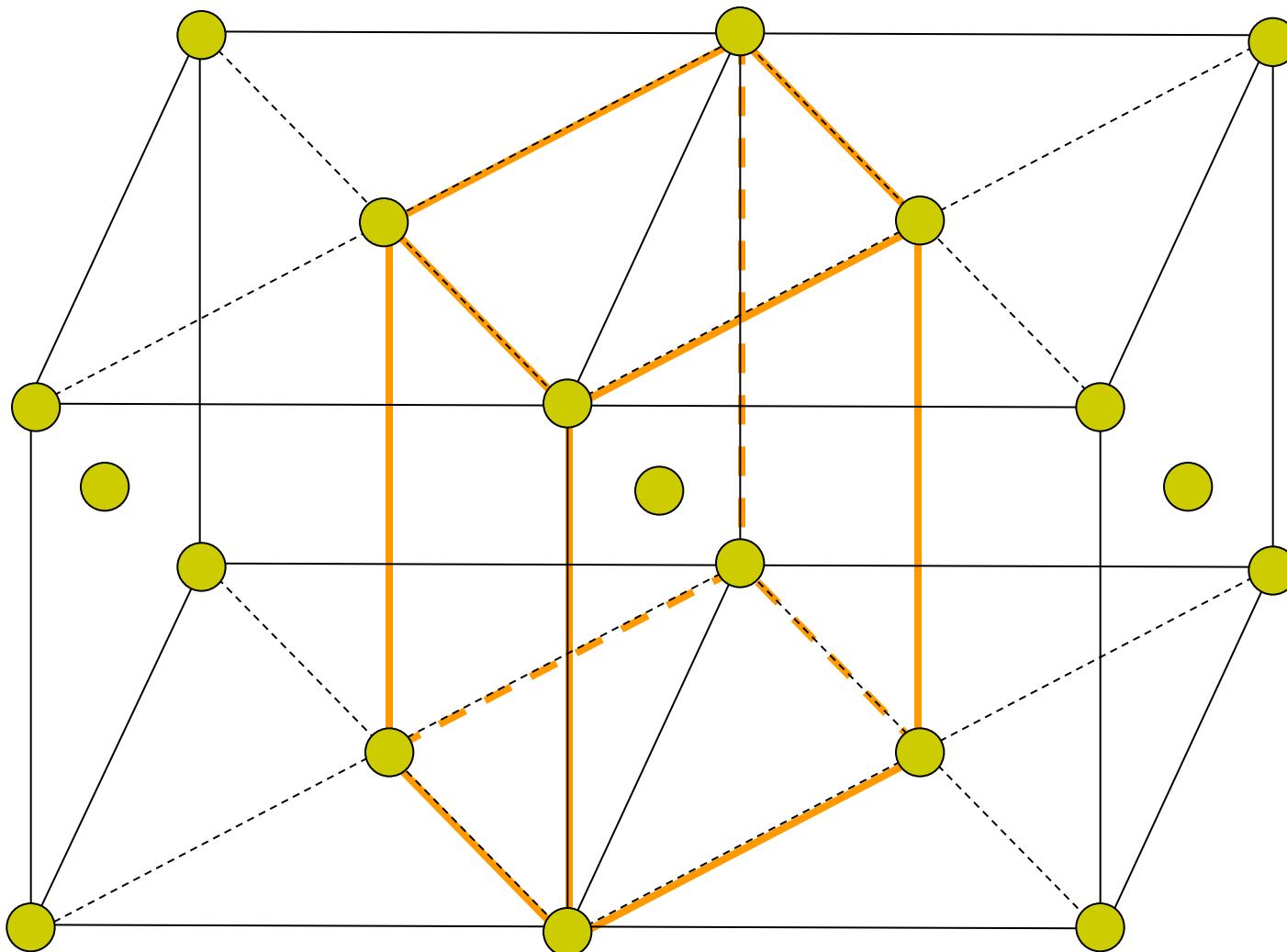
14 Bravais lattices divided into seven crystal systems

Crystal system	Bravais lattices			
1. Cubic	P	I	F	C
2. Tetragonal	P	I		
3. Orthorhombic	P	I	F	C
4. Hexagonal	P			
5. Trigonal	P			
6. Monoclinic	P			C
7. Triclinic	P			
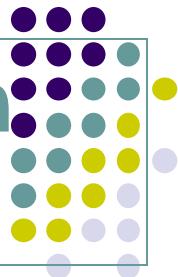
Face-centred cubic in the Bravais list ?

Cubic F = Tetragonal I
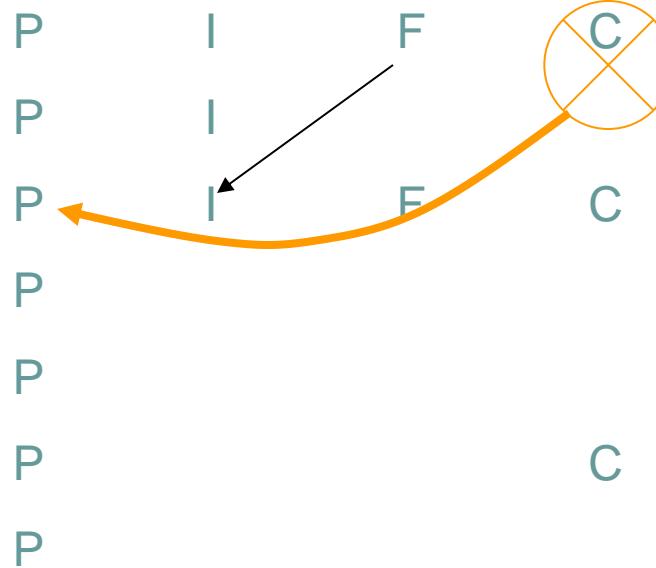
14 Bravais lattices divided into seven crystal systems
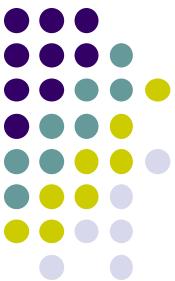
Crystal system	Bravais lattices			
1. Cubic	P	I	F	C
2. Tetragonal	P	I		
3. Orthorhombic	P	I	F	C
4. Hexagonal	P			
5. Trigonal	P			
6. Monoclinic	P			C
7. Triclinic	P			

ML **Frankenheim**

Auguste Bravais

1811-1863

Couldn't
find his
photo

Your photo

15 lattices   14 lattices   13 lattices

What is the basis for classification of lattices into

7 crystal systems
and
14 Bravais lattices?

Symmetry classification of lattices

Based on rotational and reflection symmetry alone $\Rightarrow$ 7 types of lattices

$\Rightarrow$ 7 crystal systems

Based on complete symmetry, i.e., rotational, reflection and translational symmetry

$\Rightarrow$ 14 types of lattices

$\Rightarrow$ 14 Bravais lattices
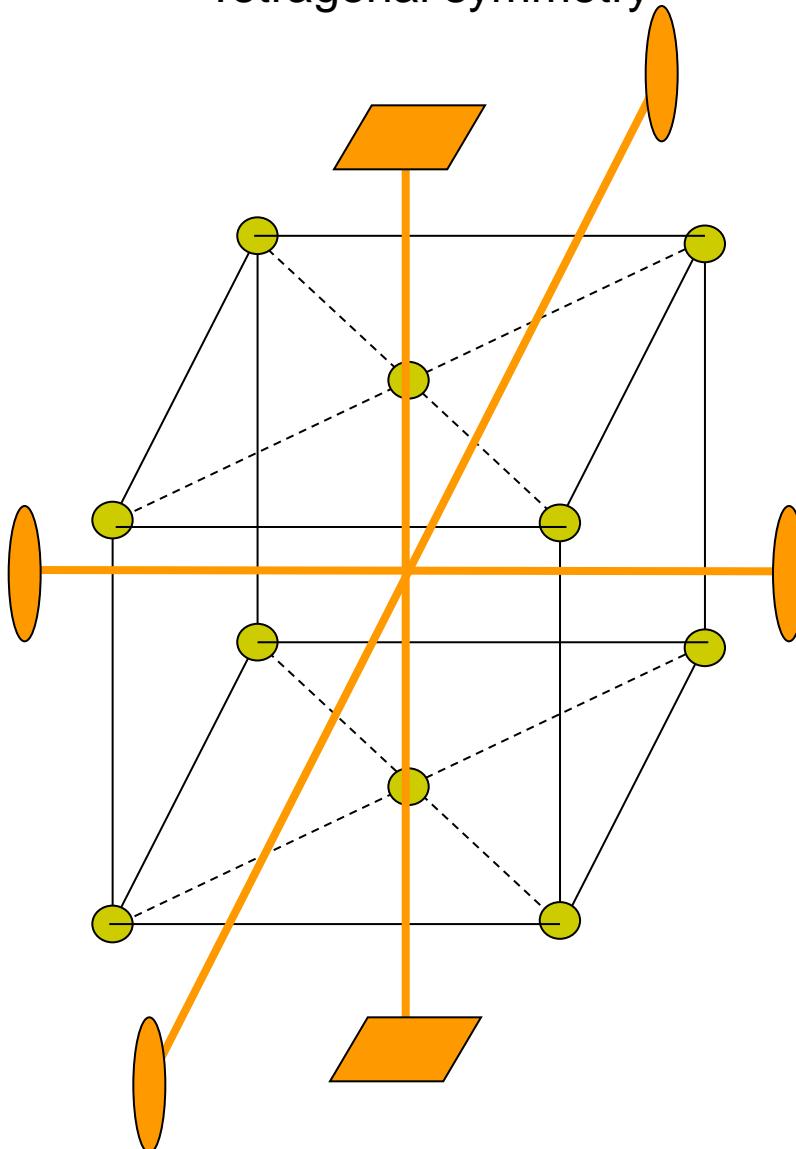
7 crystal Systems

System	Required symmetry
• Cubic	Three 4-fold axis
• Tetragonal	one 4-fold axis
• Orthorhombic	three 2-fold axis
• Hexagonal	one 6-fold axis
• Rhombohedral	one 3-fold axis
• Monoclinic	one 2-fold axis
• Triclinic	none
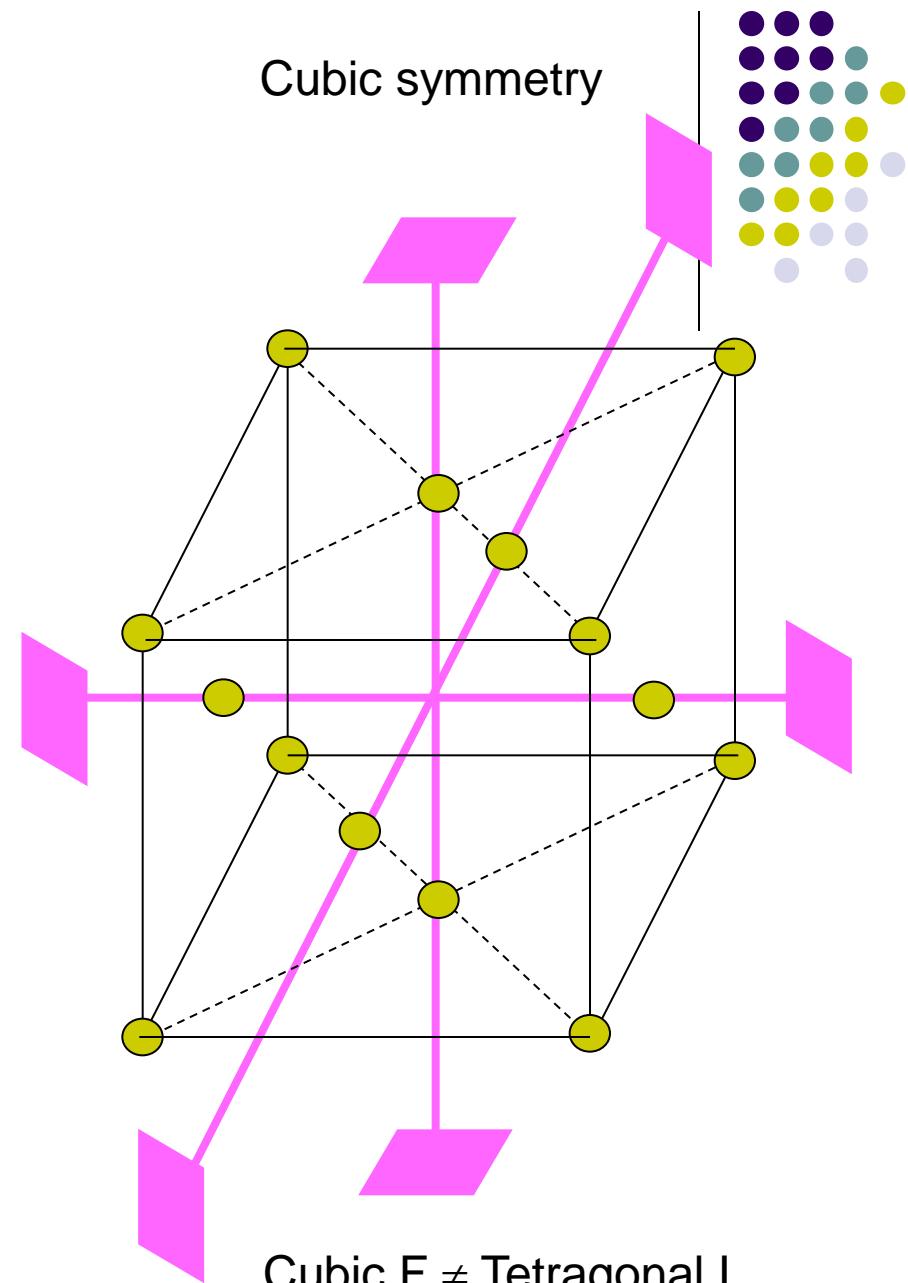
Tetragonal symmetry
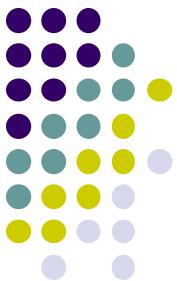
Cubic symmetry

Cubic C = Tetragonal P

Cubic F $\neq$ Tetragonal I

Notation

P: Primitive (lattice points only at the corners of the unit cell)

I: Body-centred (lattice points at the corners + one lattice point at the centre of the unit cell)

F: Face-centred (lattice points at the corners + lattice points at centres of all faces of the unit cell)

C: End-centred or base-centred (lattice points at the corners + two lattice points at the centres of a pair of opposite faces)

Crystal Systems

Crystal system	Example
Triclinic	$K_2S_2O_8, K_2Cr_2O_7$
Monoclinic	As_4S_4, KNO_2, $CaSO_4.2H_2O$, β-S
Rhombohedral	Hg, Sb, As, Bi, $CaCO_3$
Hexagonal	Zn, Co, Cd, Mg, Zr, NiAs
Orthorhombic	Ga, Fe_3C, α-S
Tetragonal	In, TiO_2, β-Sn
Cubic	Au, Si, Al, Cu, Ag, Fe, NaCl
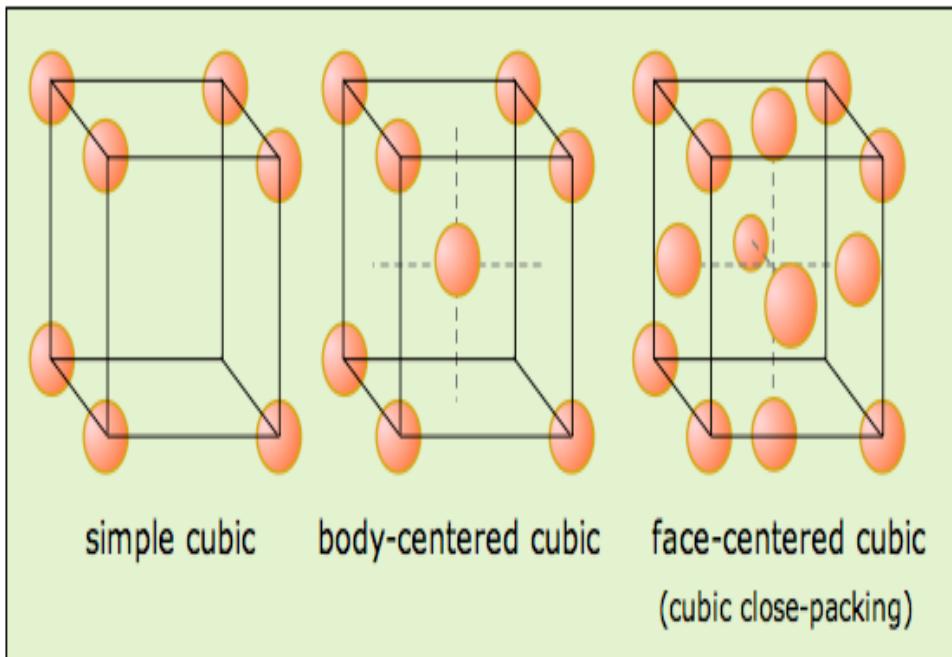
Unit cells

- Primitive unit cell:

  When atoms in unit cell are present only at the corners

- Centred Unit Cells:

  When atoms are present at other positions in addition to corners in a unit cell

simple cubic   body-centered cubic   face-centered cubic (cubic close-packing)

Coordination Number
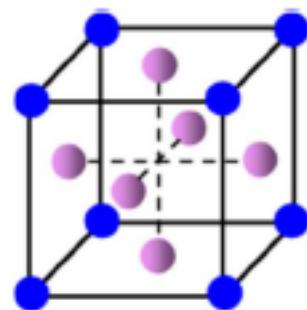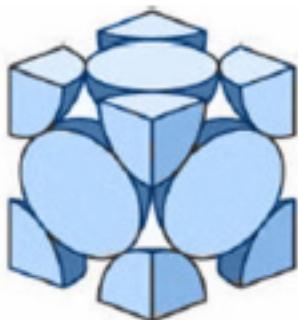
- Coordination number is the number of nearest neighbor to a particular atom in the crystal

- For example **Coordination number** for different unit cells are:

  - Simple cubic – 6

  - Body centered – 8

  - Face centered --12

Coordination number
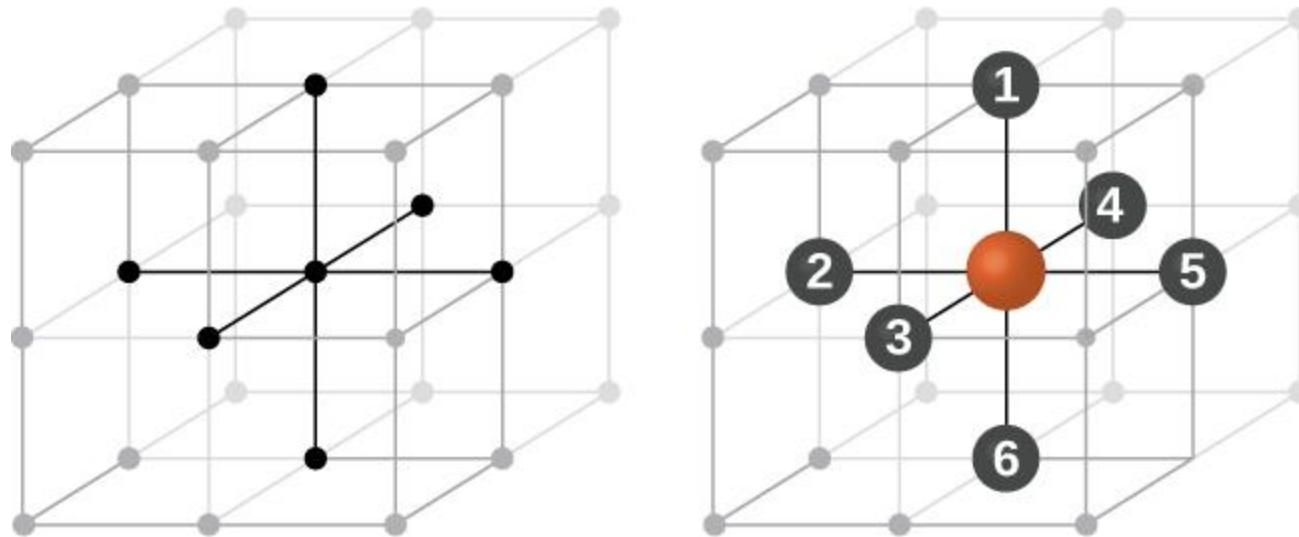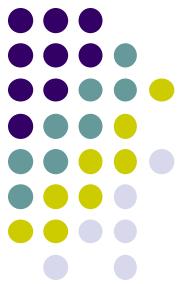
Coordination number is the number of nearest neighbor to a particular atom in the crystal


In the FCC lattice each atom is in contact with 12 neighbor atoms. FCC coordination number Z = 12
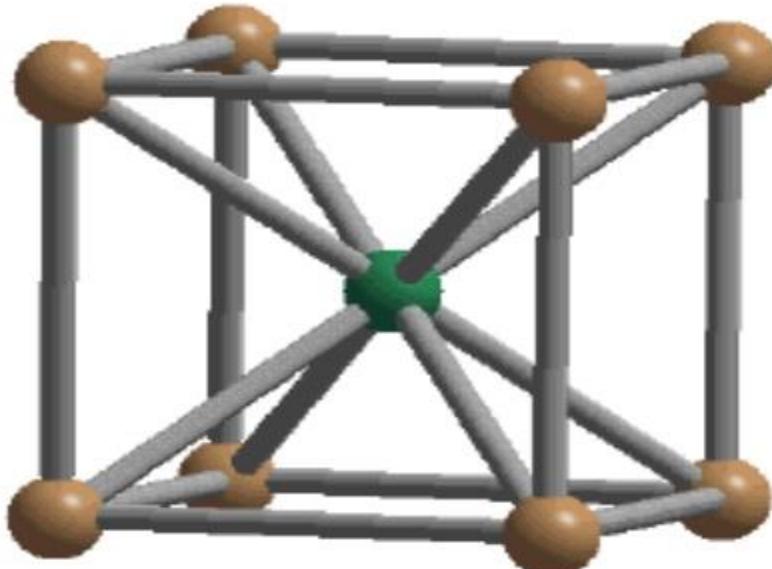
For example, the face centered atom in the front face is in contact with four corner atoms and four other face-centered atoms behind it (two sides, top and bottom) and is also touching four face-centered atoms of the unit cell in front of it.

Coordination Number of Simple Cubic
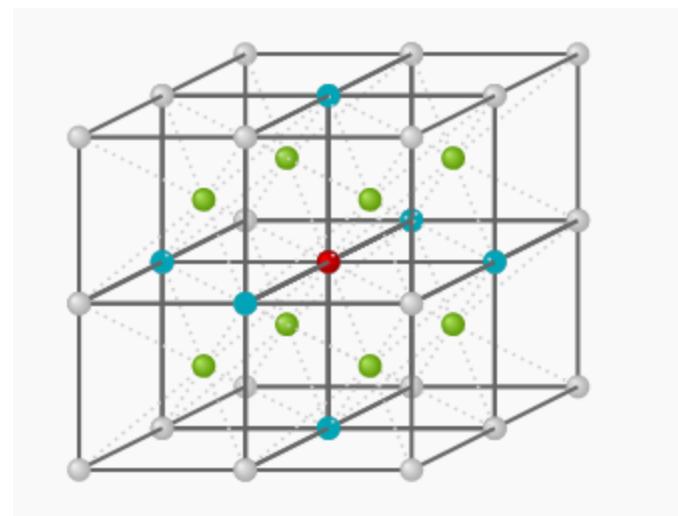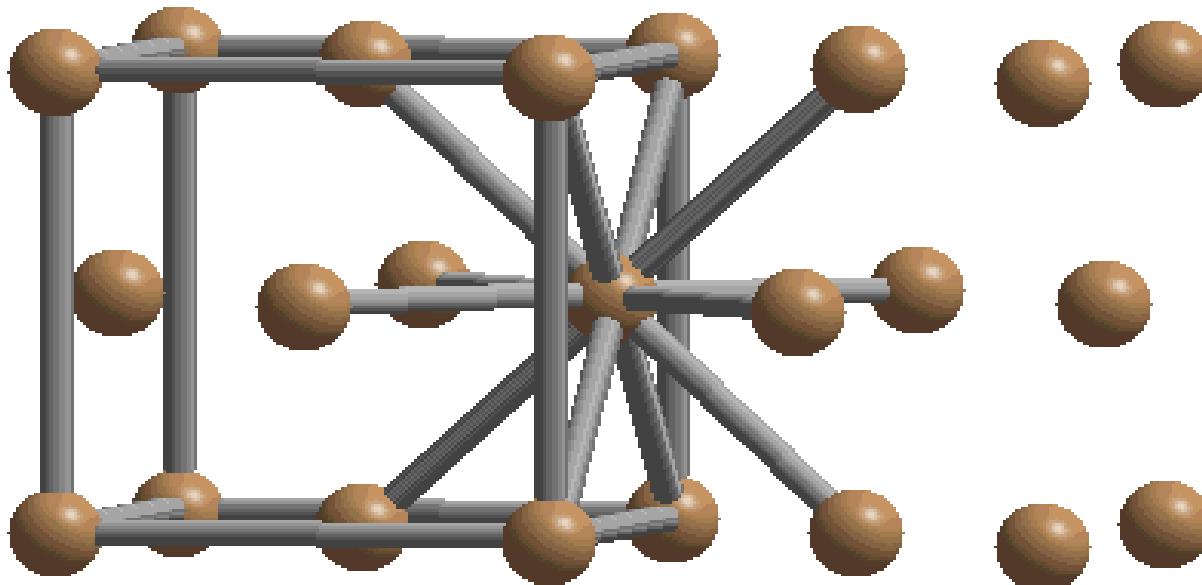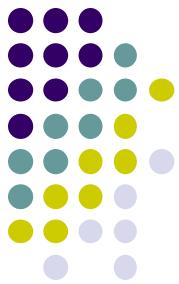
# Coordination Number of BCC


Hari Prasad

Coordination Number of FCC
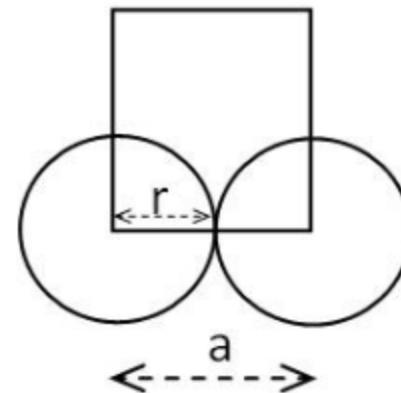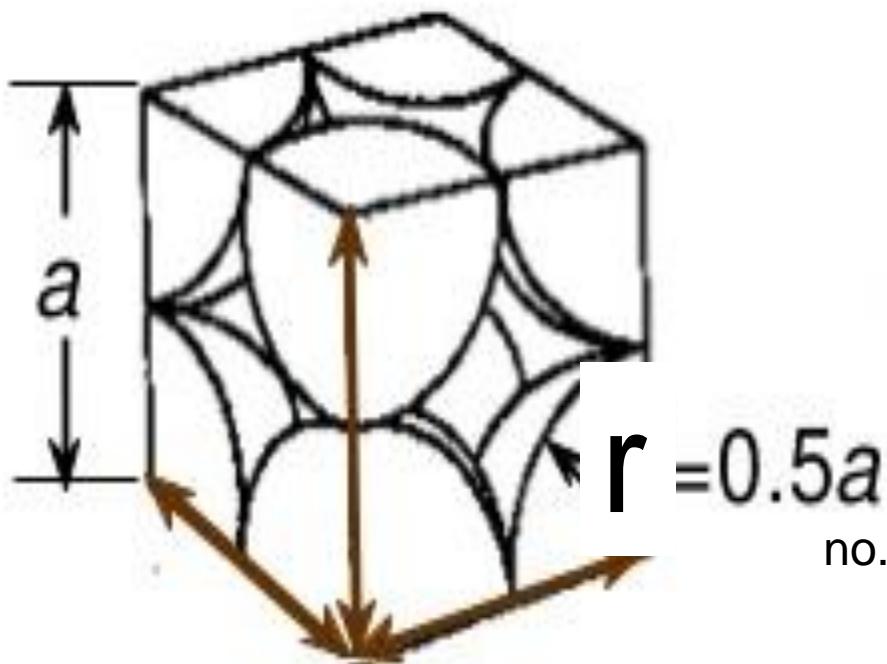
Atomic Packing efficiency

- Packing efficiency indicates how closely atoms are packed in a unit cell

$$APF = \frac{Volume\ of\ atoms\ in\ unit\ cell}{Volume\ of\ unit\ cell}$$

Atomic Packing efficiency of Simple Cubic

$r = 0.5a$
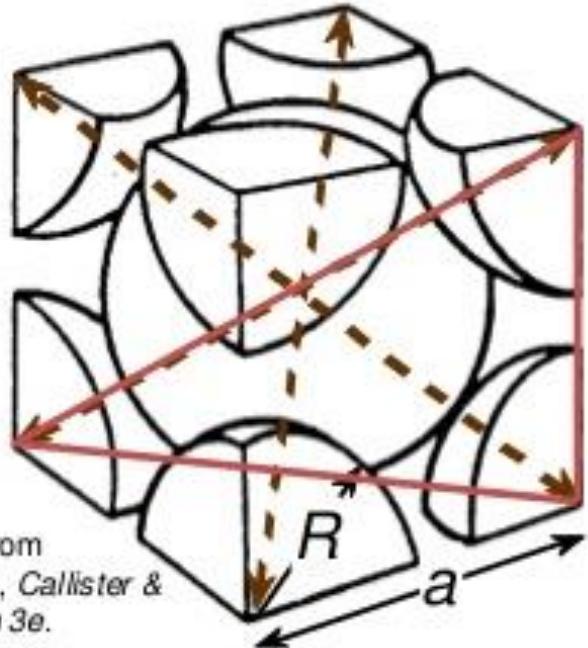
no. of atoms per unit cell = (1/8)*8 =1.
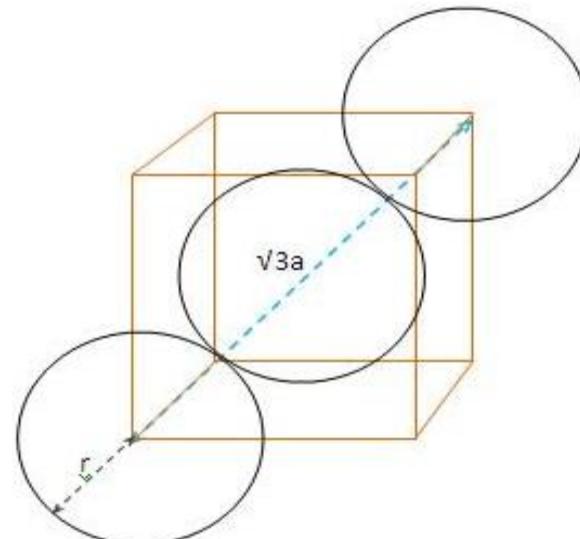
Volume of unit cell = $a^3 = (2r)^3 = 8r^3$

$$APF = \frac{\frac{4}{3}\pi r^3}{8r^3} = \frac{\pi}{6} = 52\%$$

Atomic Packing efficiency of BCC
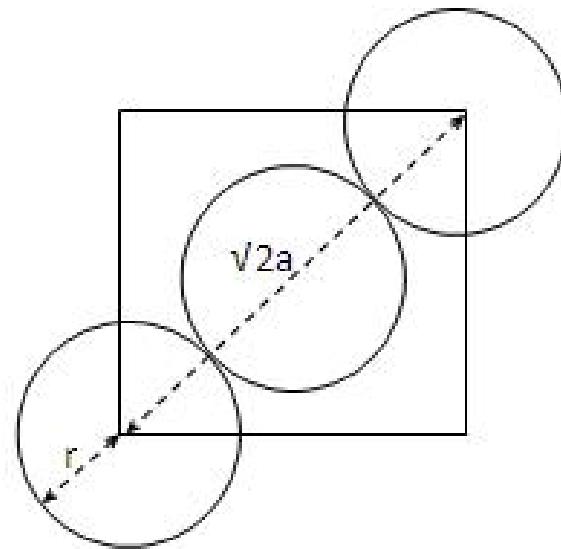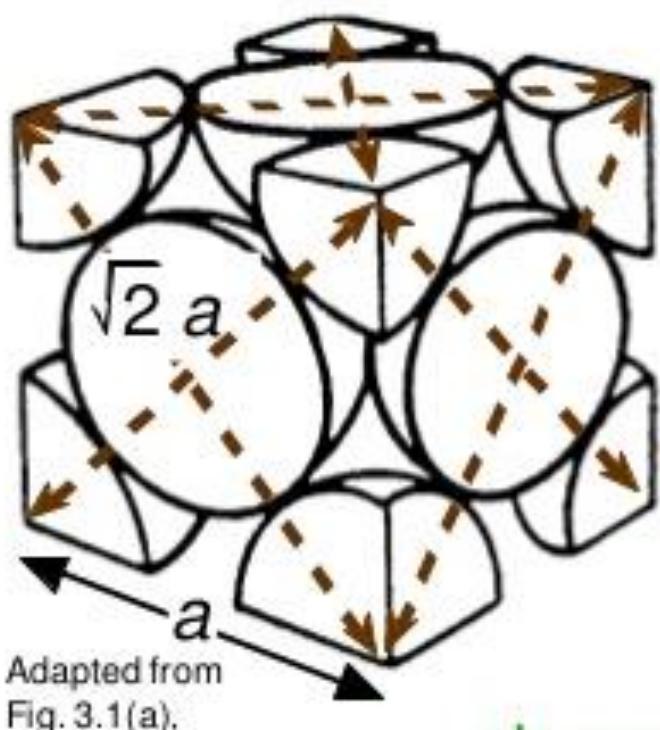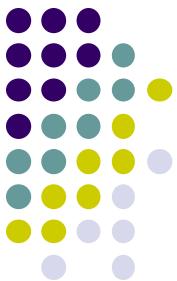
Adapted from
Fig. 3.2(a), *Callister &
Rethwisch* 3e.

$\sqrt{3}a$

no. of atoms per unit cell=
(1/8)*8(corner atoms)+1(body centre)=2.

$$APF = \frac{\frac{8\pi r^3}{3}}{\frac{64 r^3}{(3\sqrt{3})}} = \frac{\sqrt{3}\,\pi}{8} = 68\%$$

Atomic Packing efficiency of FCC
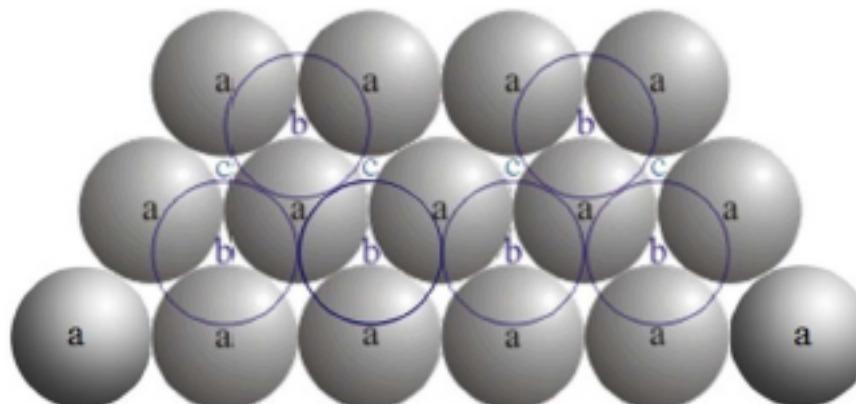
no. of atoms per unit cell is=(1/8)*8(corner atoms)+(1/2)*6(atoms at face)=4

$$APF = \frac{\frac{16}{3}\pi r^3}{(\frac{4r}{\sqrt{2}})^3} = \frac{\pi}{3\sqrt{2}} = 74\%$$

Adapted from Fig. 3.1(a).

Close-Packed Structure

➤FCC and hexagonal crystal structures are most highly packed with packing efficiency of 74% (APF= 0.74). Such structures can be described in terms of close-packed atomic planes.

➤In FCC, {111} planes are close-packed and the basal plane (0001) is the close-packed one in hexagonal close-packed (HCP) system. Therefore, both of these structures can be generated by stacking of these planes. A portion of such a stack is shown in the picture below.

Close-Packed Structure
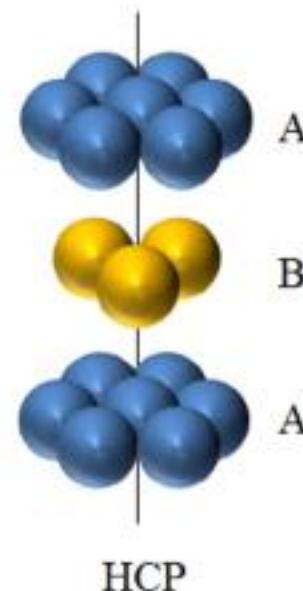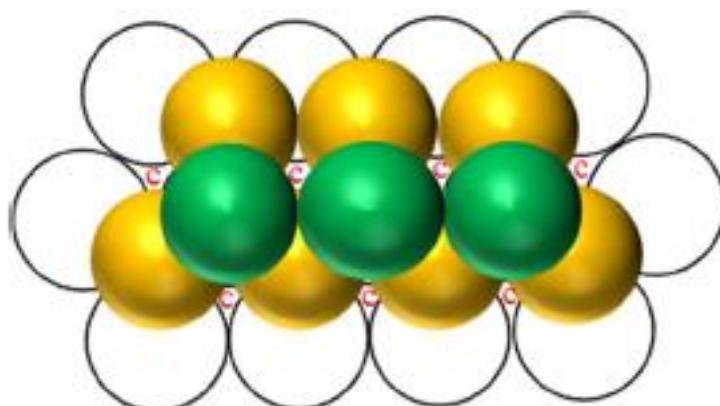
➤ There are two types of voids between the atoms – vertex up (*b*), and vertex down (*c*). The atoms in the next layer sit on the *b* sites (See animation below).

➤ In FCC, atoms in the third layer sit over the *c* sites and this repeats giving rise to ABC ABC ABC type of stacking.

Close-Packed Structure

➢In HCP system, centers of atoms of the third layer lie directly over centers of atoms of the first layer (**a** positions) giving rise to AB AB AB type of stacking.

HCP

Structure-Property correlation

Aluminium (Al) is ductile while iron (Fe) and magnesium (Mg) are not. This can be explained from their crystal structures.

Al is FCC where as Fe is BCC and Mg is HCP.

Plastic deformation in metals takes place mainly by a process called slip. Slip can broadly be visualized as sliding of crystal planes over one another. Slip occurs on most densely packed planes in the most closely packed directions lying on that plane.

The slip plane and the direction together is called a
Slip system

Structure-Property correlation

❑In FCC, {111} planes are close-packed and there are four unique {111} planes. Each of these planes contains three closely packed <110> directions. Therefore, there are 4 x 3 = 12 slip systems

❑In HCP, the basal plane, (0001) is the close-packed and it contains three <1 1 $\bar{2}$ 0> directions. Hence, number of slip system = 1 x 3 = 3

❑Slip in more number of slip systems allows greater plastic deformation before fracture imparting ductility to FCC materials