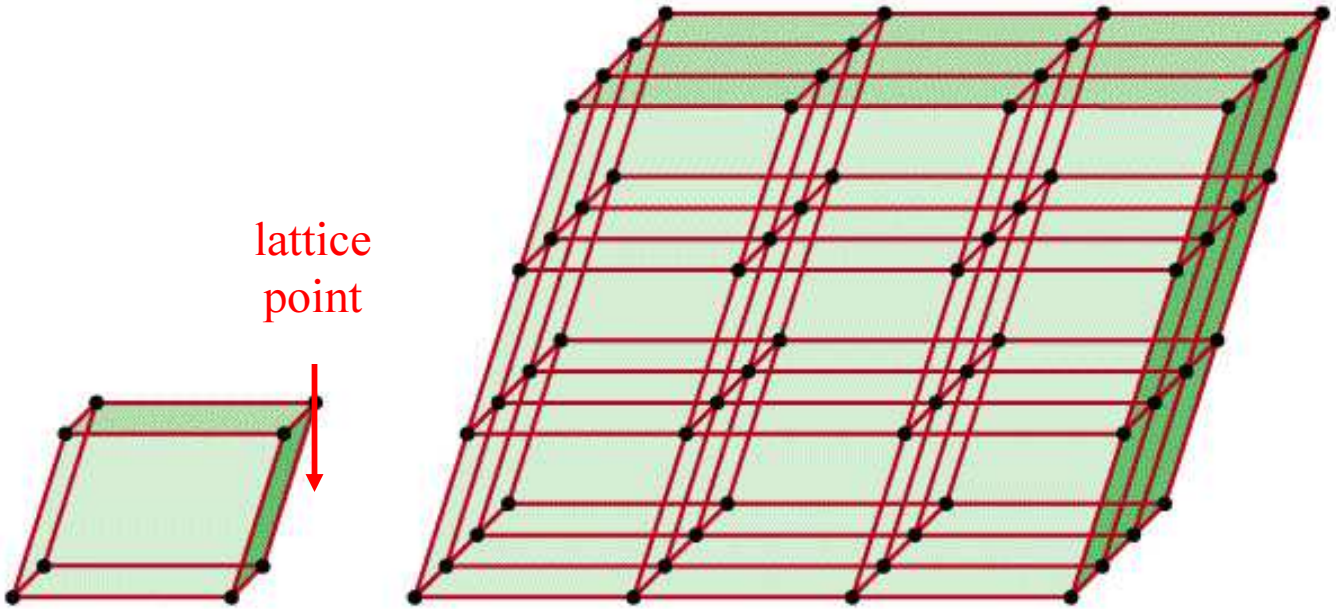
A ***crystalline solid*** possesses rigid and long-range order. In a crystalline solid, atoms, molecules or ions occupy specific (predictable) positions.

An ***amorphous solid*** does not possess a well-defined arrangement and long-range molecular order.

A ***unit cell*** is the basic repeating structural unit of a crystalline solid.



Unit Cell

Unit cells in 3 dimensions

<u>At lattice points:</u>

- Atoms
- Molecules
- Ions

Crystal = Lattice + Motif

Motif or Basis:
an entity (typically an atom or a group of atoms) associated with each lattice point

Lattice ➢ the underlying periodicity of the crystal
Motif ➢ Entity associated with each lattice points

Lattice ➢ how to repeat
Motif ➢ what to repeat

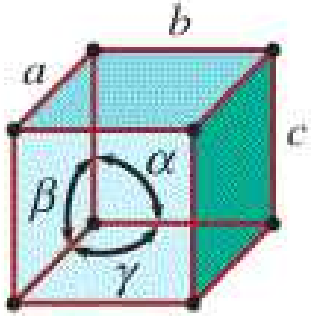
Lattice

Translationally periodic arrangement of points

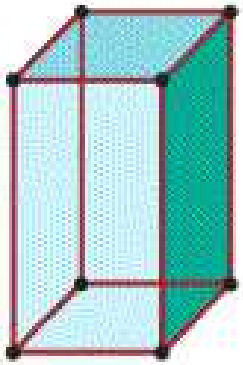
Crystal

Translationally periodic arrangement of motifs

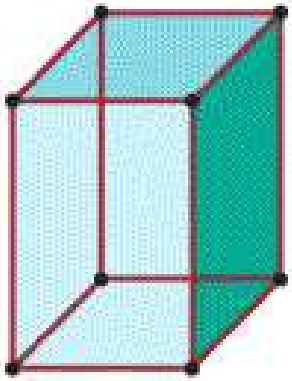
Seven Types of Unit Cells



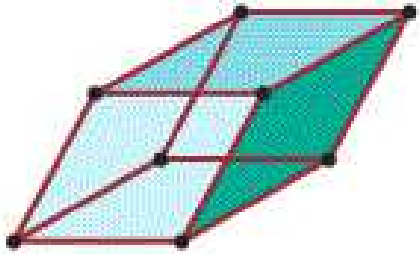
Simple cubic
$a = b = c$
$\alpha = \beta = \gamma = 90^\circ$



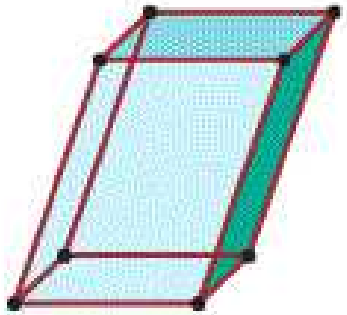
Tetragonal
$a = b \neq c$
$\alpha = \beta = \gamma = 90^\circ$



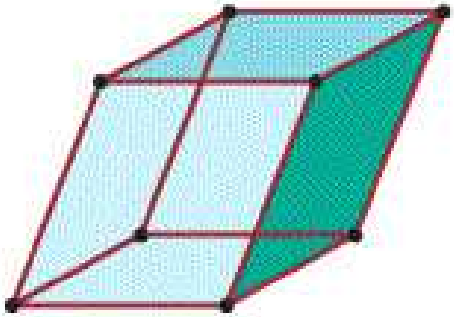
Orthorhombic
$a \neq b \neq c$
$\alpha = \beta = \gamma = 90^\circ$



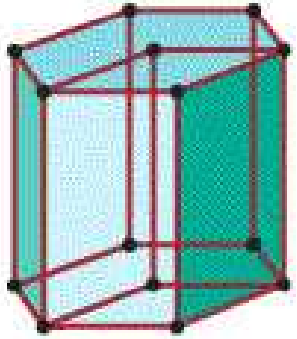
Rhombohedral
$a = b = c$
$\alpha = \beta = \gamma \neq 90^\circ$



Monoclinic
$a \neq b \neq c$
$\alpha = \gamma = 90^\circ, \beta \neq 90^\circ$

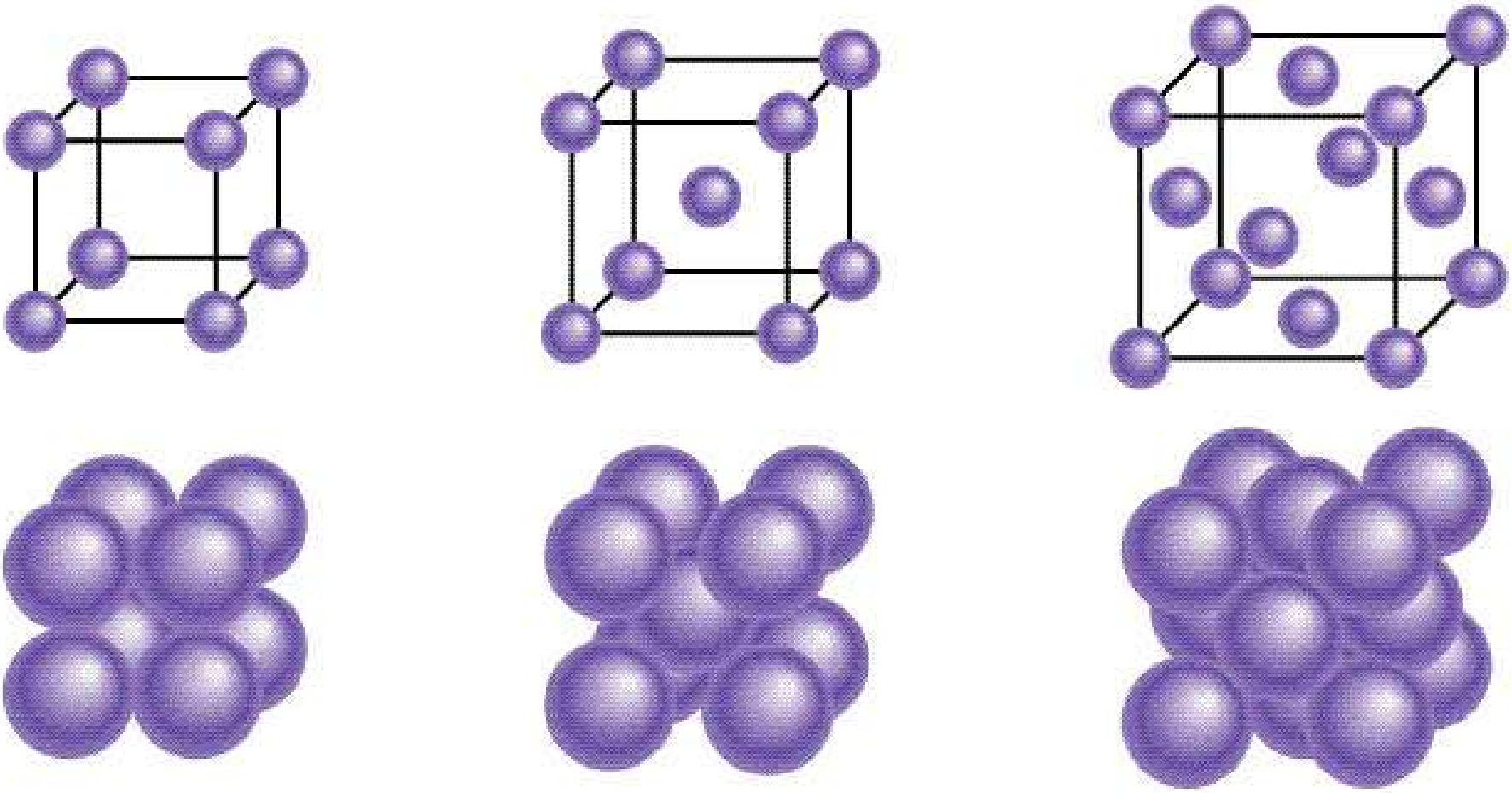


Triclinic
$a \neq b \neq c$
$\alpha \neq \beta \neq \gamma \neq 90^\circ$



Hexagonal
$a = b \neq c$
$\alpha = \beta = 90^\circ, \gamma = 120^\circ$

Three Types of Cubic Cells

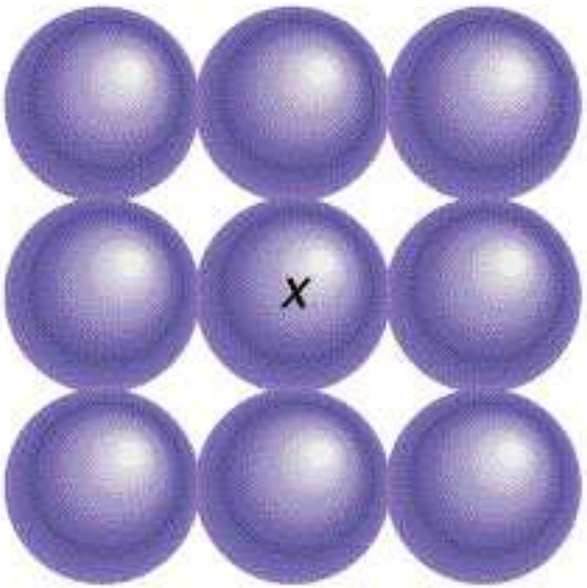


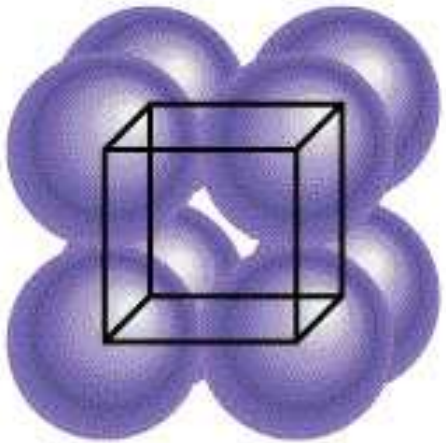
Simple cubic

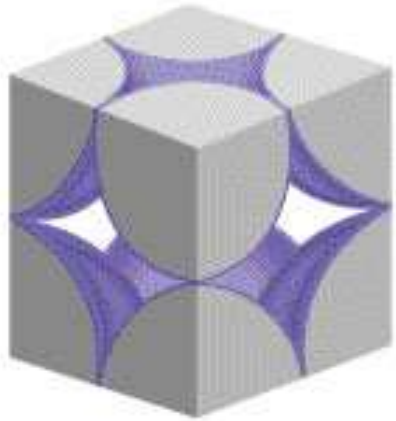
Body-centered cubic

Face-centered cubic

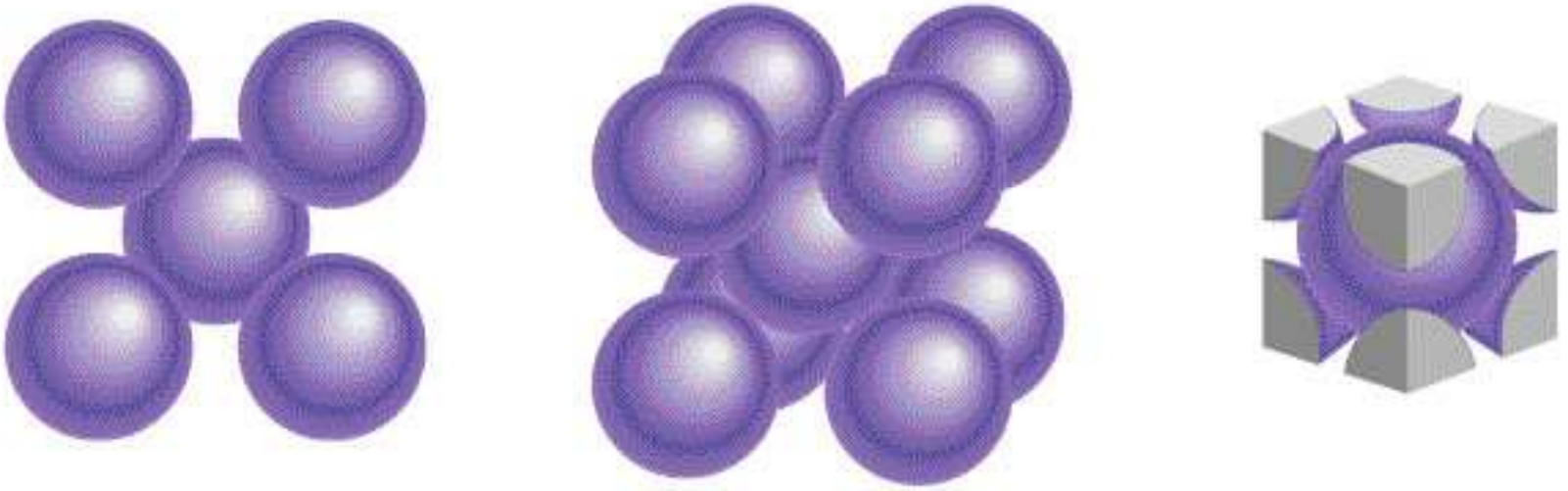
Arrangement of Identical Spheres in a simple Cubic Cell



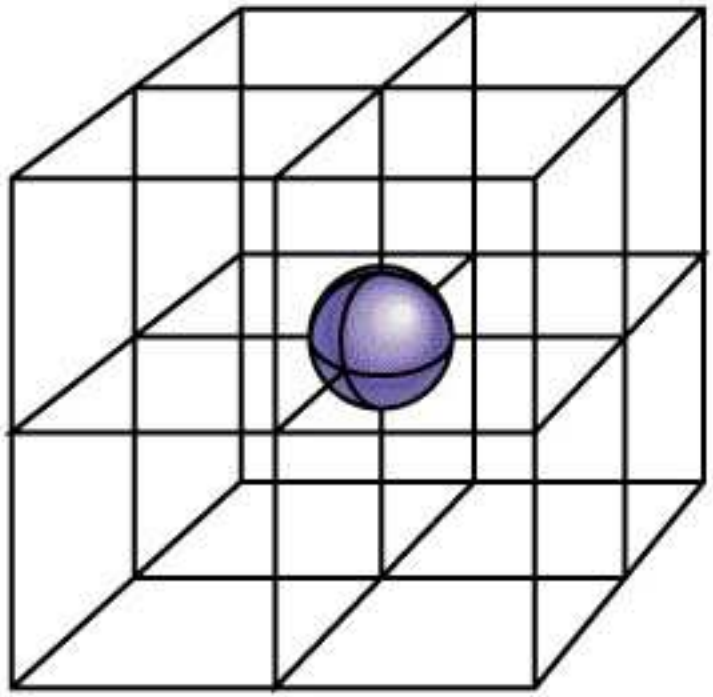




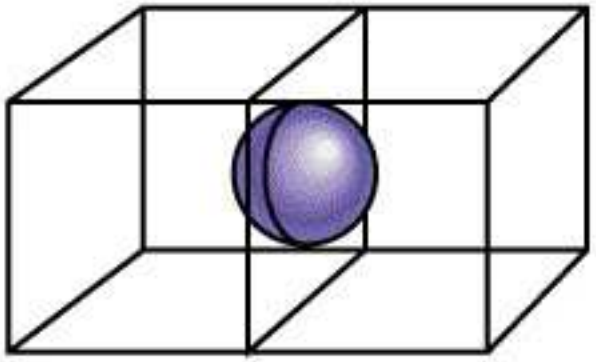
Arrangement of Identical Spheres in a Body-Centered Cube



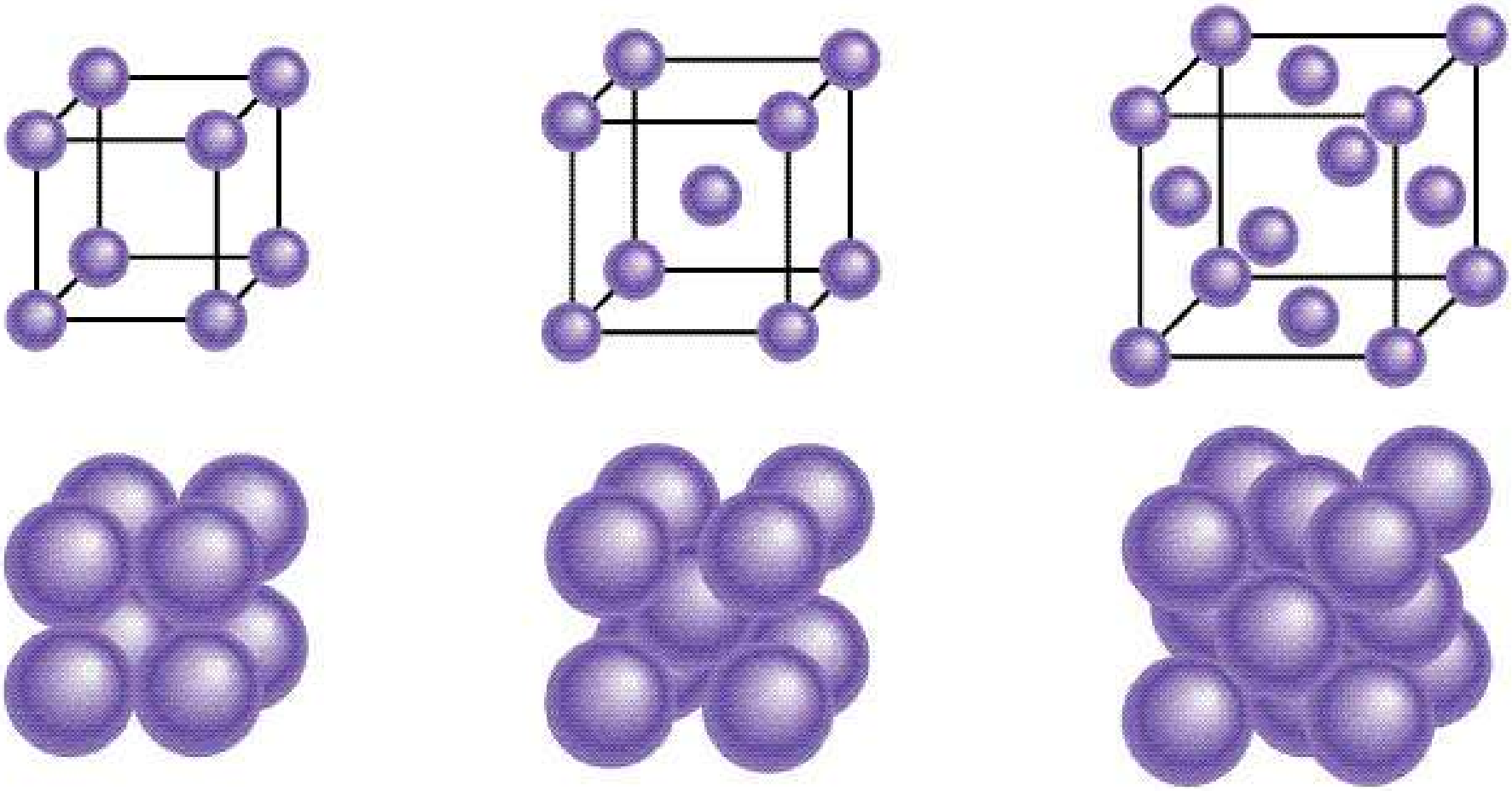
A Corner Atom and a Face-Centered Atom



Shared by 8 unit cells



Shared by 2 unit cells



Simple cubic

1 atom/unit cell

(8 x 1/8 = 1)

Body-centered cubic

2 atoms/unit cell

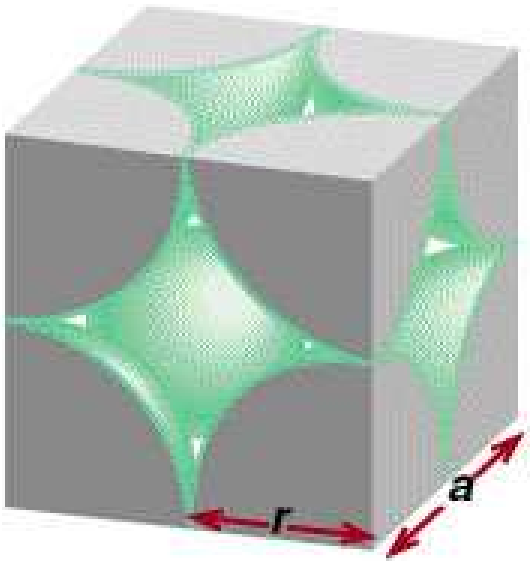
(8 x 1/8 + 1 = 2)

Face-centered cubic

4 atoms/unit cell

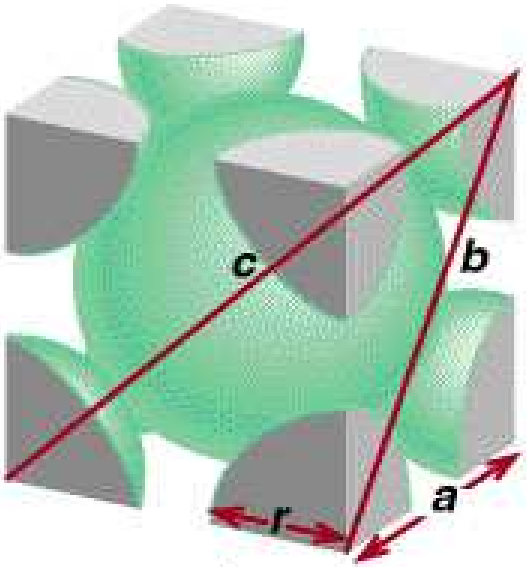
(8 x 1/8 + 6 x 1/2 = 4)

Relationship Between the Atomic Radius and the Edge Length in Three Different Unit Cells



scc

$a = 2r$



bcc

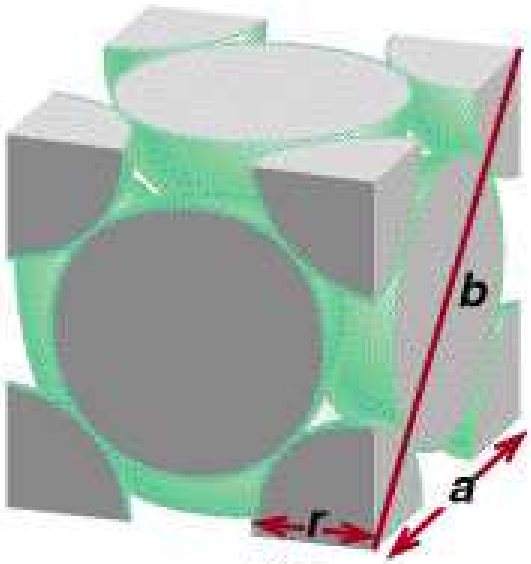
$b^2 = a^2 + a^2$

$c^2 = a^2 + b^2$

$= 3a^2$

$c = \sqrt{3}a = 4r$

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



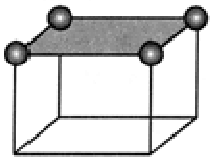
fcc

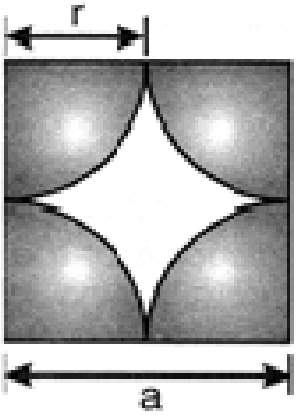
$b = 4r$

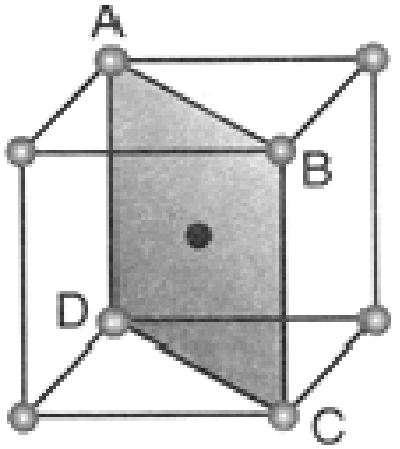
$b^2 = a^2 + a^2$

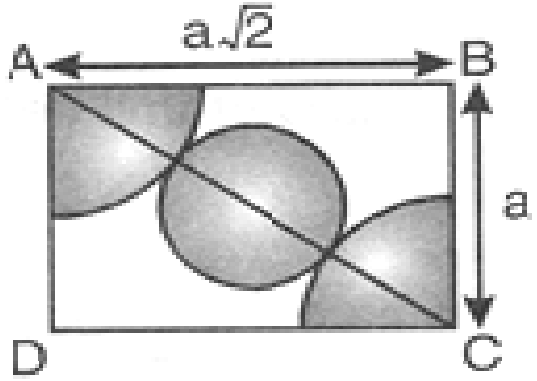
$16r^2 = 2a^2$

$a = \sqrt{8}r$




r
a

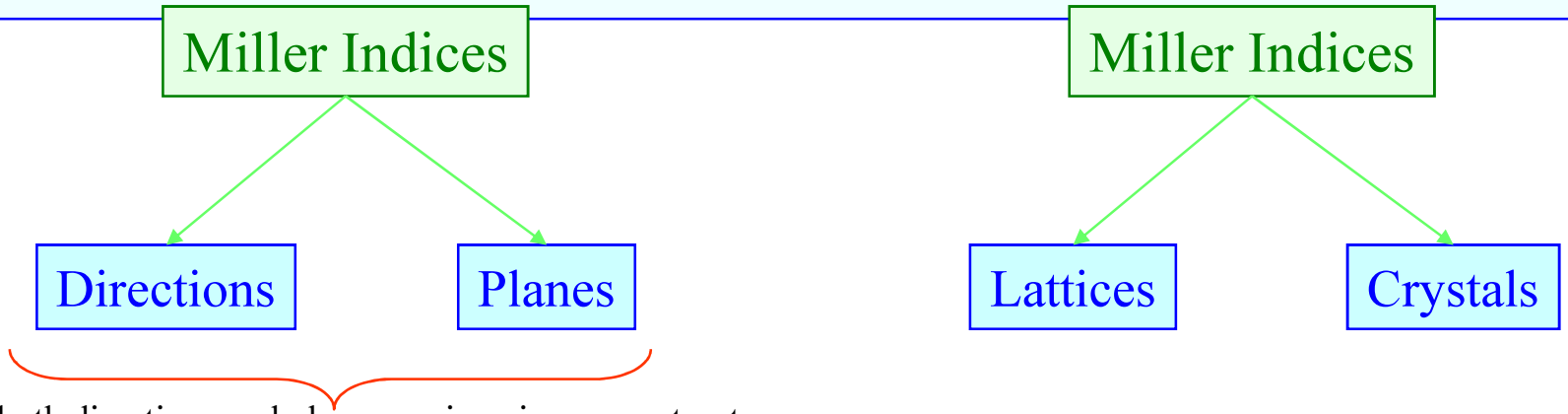

A
B
D
C


a√2
A
B
a
D
C

Property	SC	BCC	FCC
Edge length, a	$a = 2r$	$a = (4/\sqrt{3})r$	$a = \sqrt{8}\ r$
Volume of unit cell	$a^3 = 8r^3$	$a^3 = (4/\sqrt{3}r)^3$	$a^3 = (2\sqrt{2}\ r)^3$
No. of Atoms per unit cell	1	2	4
Volume occupied by atoms per unit cell	1 x (4/3) pi r^3	2 x (4/3) pi r^3	4 x(4/3) pi r^3
Packing Fraction = $\frac{\text{vol. occupied by atoms}}{\text{vol. of unit cell}}$	= 0.524	= 0.68	= 0.74
% Free space per unit cell	47.6%	26%	32%

MILLER INDICES

- Miller indices are used to specify directions and planes.
- These directions and planes could be in lattice or in crystals.
- *(It should be mentioned at the outset that special care should be given to see if the indices are in a lattice or a crystal).*
- The number of indices will match with the dimension of the lattice or the crystal: in 1D there will be 1 index and 2D there will be two indices etc.
- Some aspects of Miller indices, especially those for planes, are not intuitively understood and hence some time has to be spent to familiarize oneself with the notation.



Note: both directions and planes are imaginary constructs

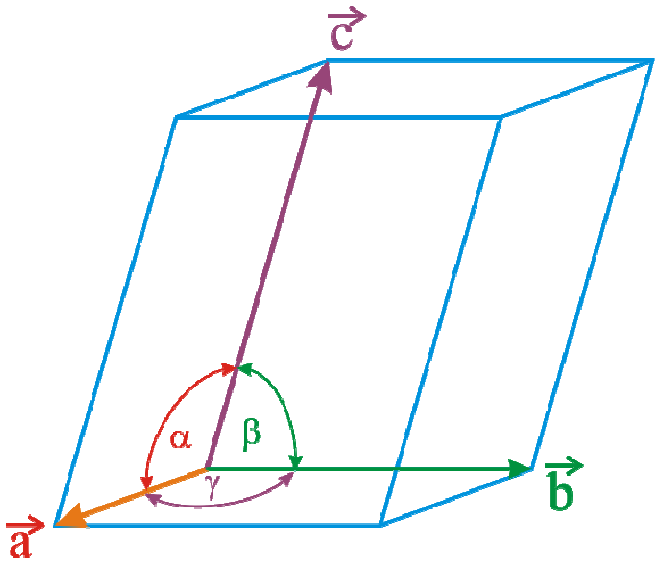
Miller indices for DIRECTIONS

A vector **r** passing from the origin to a lattice point can be written as: $\mathbf{r} = r_1\,\mathbf{a} + r_2\,\mathbf{b} + r_3\,\mathbf{c}$

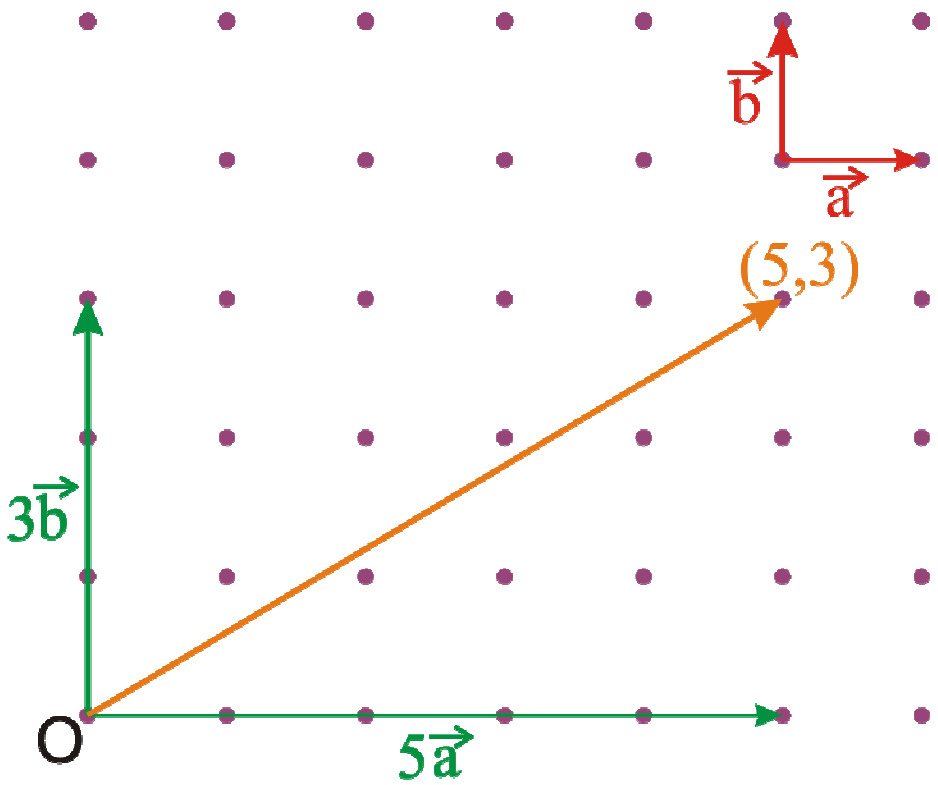
$$r = r_1\,\vec{a} + r_2\,\vec{b} + r_3\,\vec{c}$$

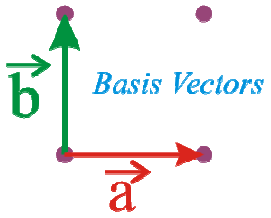
Where, **a**, **b**, **c** → basis vectors

- Basis vectors are unit lattice translation vectors which define the coordinate axis *(as in the figure below)*.
- *Note their length is not 1 unit! (like for the basis vectors of a coordinate axis).*



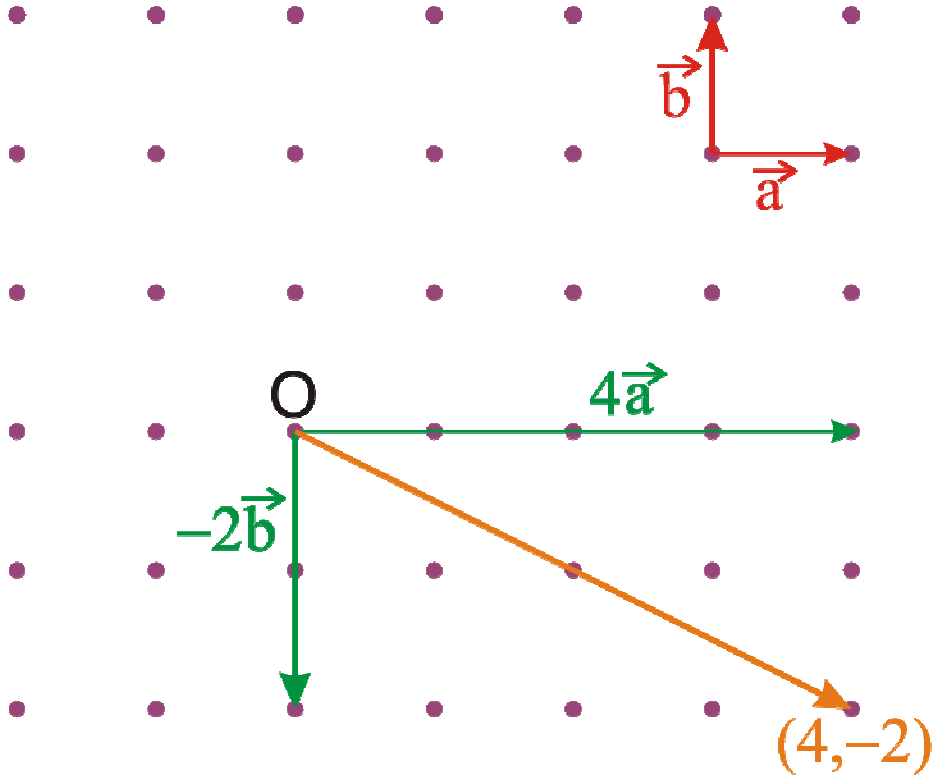
Miller Indices for directions in 2D





Miller indices → [53]

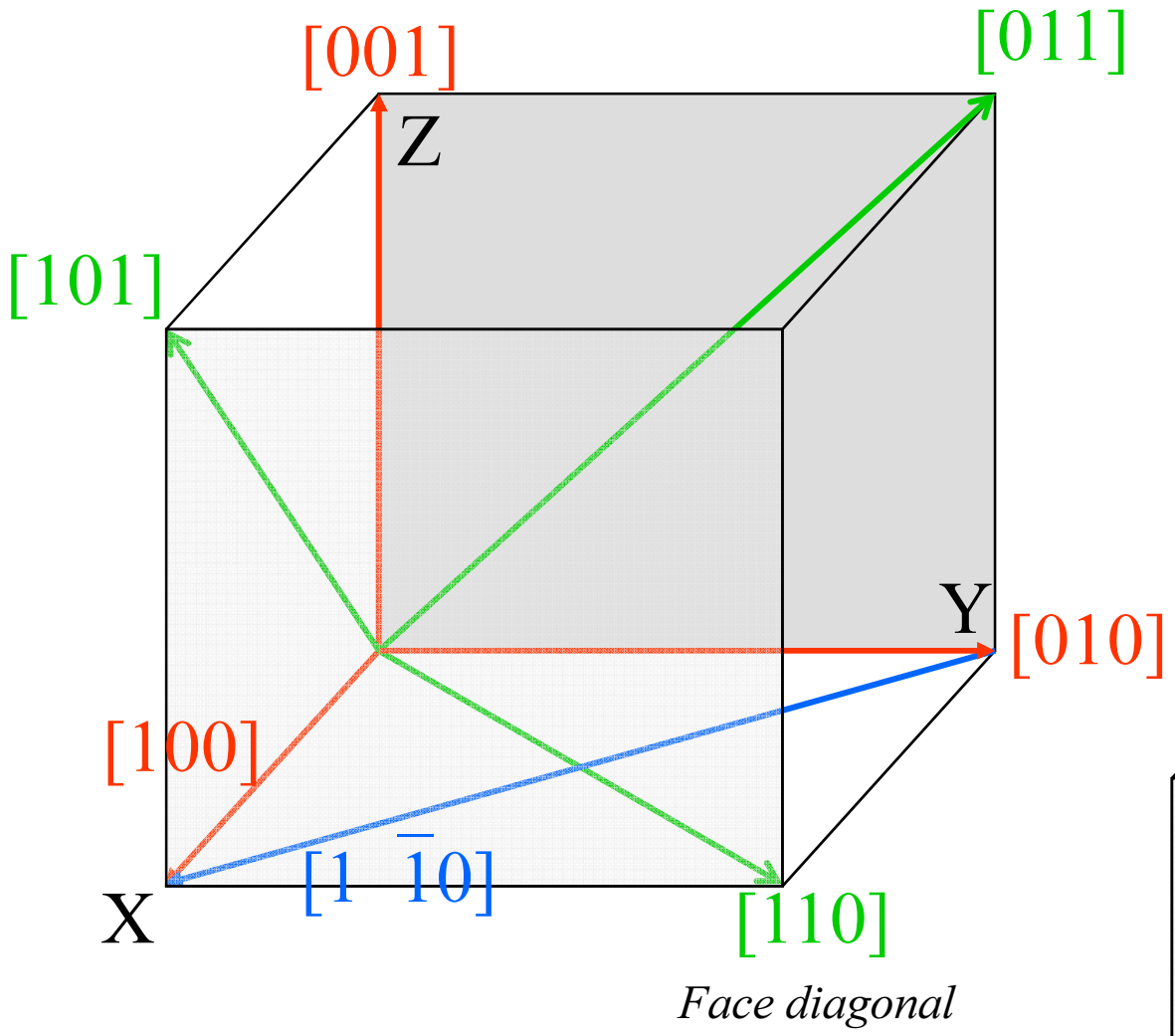
Another 2D example

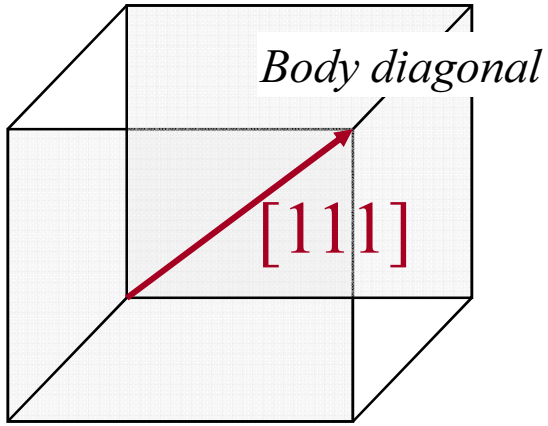


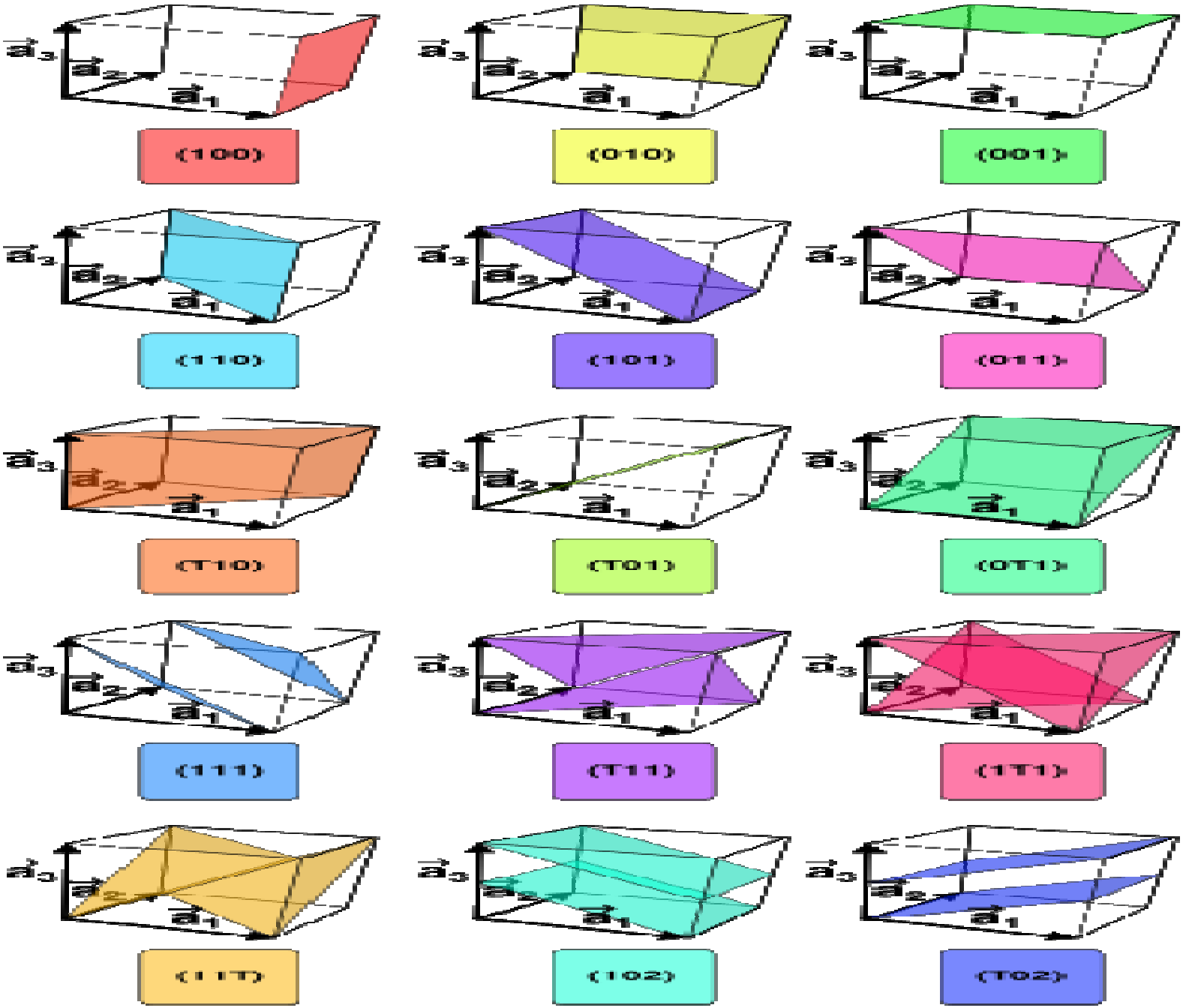
Miller Indices for the direction with magnitude $\rightarrow 2[2\,\bar{1}]$

Miller Indices for just the direction $\rightarrow [2\,\bar{1}]$

Important directions in 3D represented by Miller Indices (cubic lattice)






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

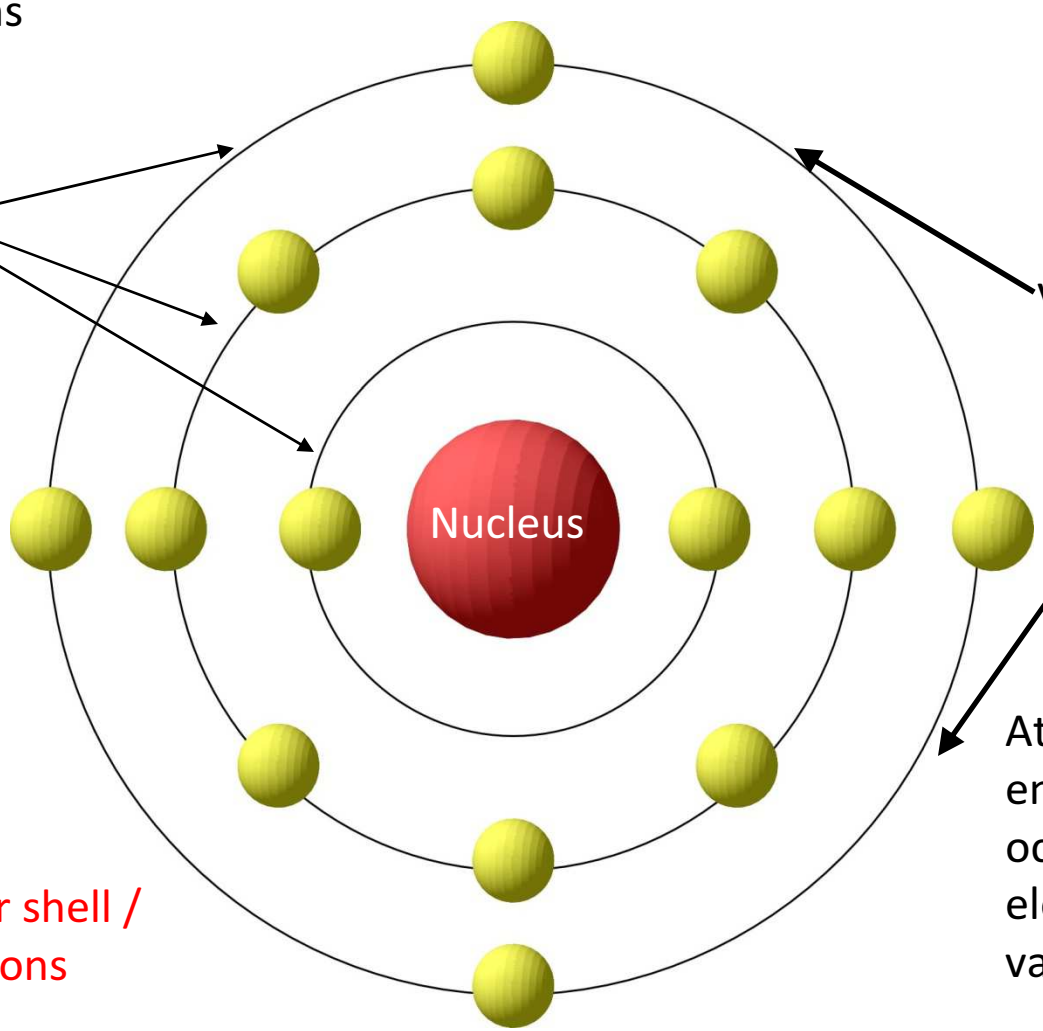
Summary of notations

	Symbol			
Direction	[ ]	[uvw]	→	Particular direction
	< >	<uvw>	→	Family of directions
Plane	( )	(hkl)	→	Particular plane
	{ }	{hkl}	→	Family of planes

Silicon

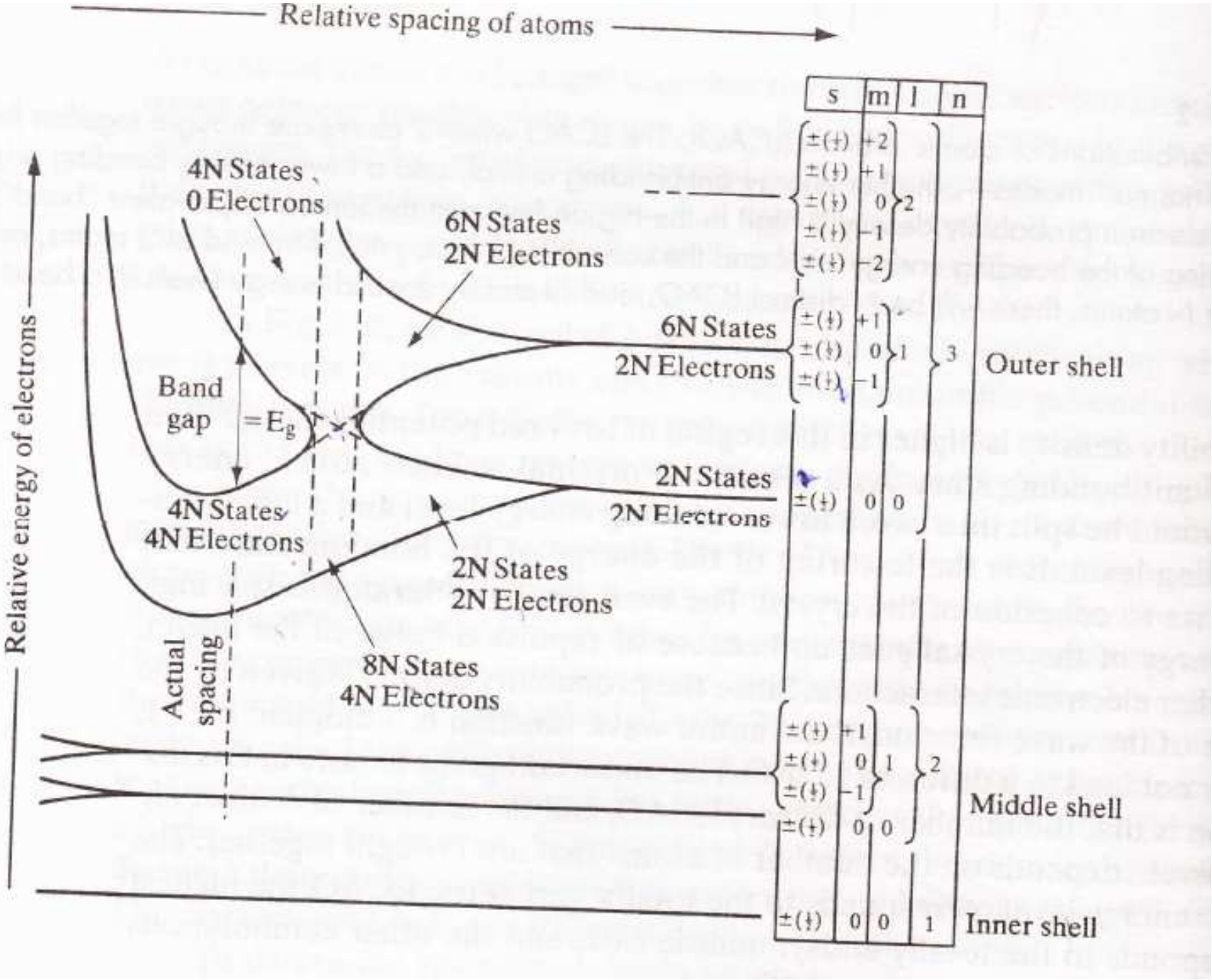
Silicon is the primary semiconductor used in VLSI systems

Si has 14 Electrons

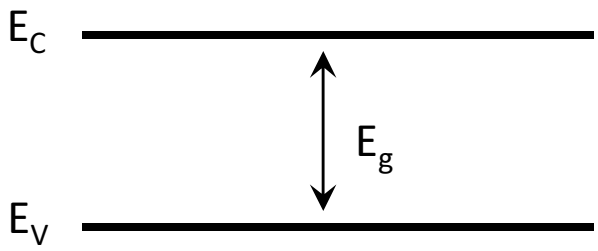


Silicon has 4 outer shell / valence electrons

At T=0K, the highest energy band occupied by an electron is called the valence band.


Relative spacing of atoms
Relative energy of electrons
4N States
0 Electrons
6N States
2N Electrons
6N States
2N Electrons
Band
gap
$= E_g$
2N States
2N Electrons
4N States
4N Electrons
2N States
2N Electrons
Actual
spacing
8N States
4N Electrons
s
m
l
n
Outer shell
Middle shell
Inner shell

Band Diagrams



Band Diagram Representation

Energy plotted as a function of position

E_C → Conduction band
→ Lowest energy state for a free electron

E_V → Valence band
→ Highest energy state for filled outer shells

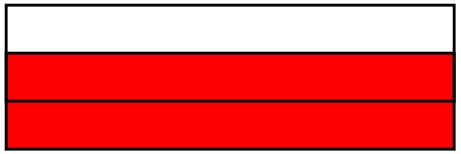
E_G → Band gap
→ Difference in energy levels between E_C and E_V
→ No electrons (e^-) in the bandgap (only above E_C or below E_V)
→ E_G = 1.12eV in Silicon

Conductor, Semiconductor or Insulator?

Examples

Silver
Copper
Gold

Overlapping Bands



- or -

Partially Filled Bands

Conductor

Silicon
Si/Ge

Semiconductor

SiO2
Diamond

Eg= 10 eV

Insulator