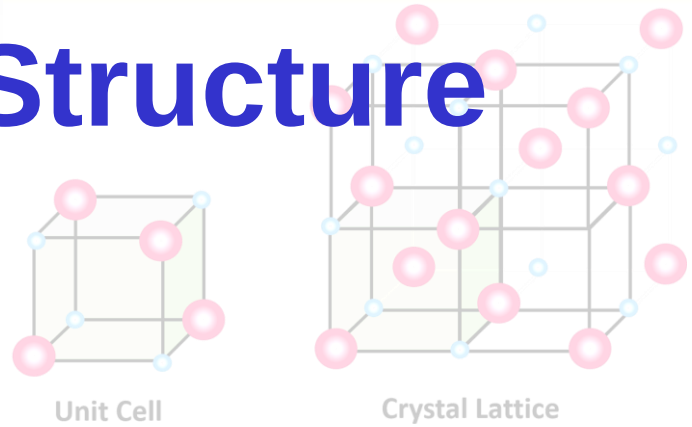
MS31007: Materials Science

Chapter 3 (Part-II): Crystal Structure



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Crystal Structure : Solid State Materials

- Lattice structures of common chemical elements.
  Concept of Bravais lattice, definition and examples.
  Primitive vectors of Bravais lattice.
  Primitive/Conventional unit cell.
- Coordination number.
- Examples of common crystal structures.
  - Body-centered cubic lattice.
  - Face-centered cubic lattice.
  - Crystal systems
  - Lattice planes and Miller indices.
- Ceramic Crystal Structures
- Determination of Lattice Spacing : X-ray Diffraction

Celestite is a mineral consisting of strontium sulfate ($SrSO_4$). Orthorhombic

Pyrite – FeS_2

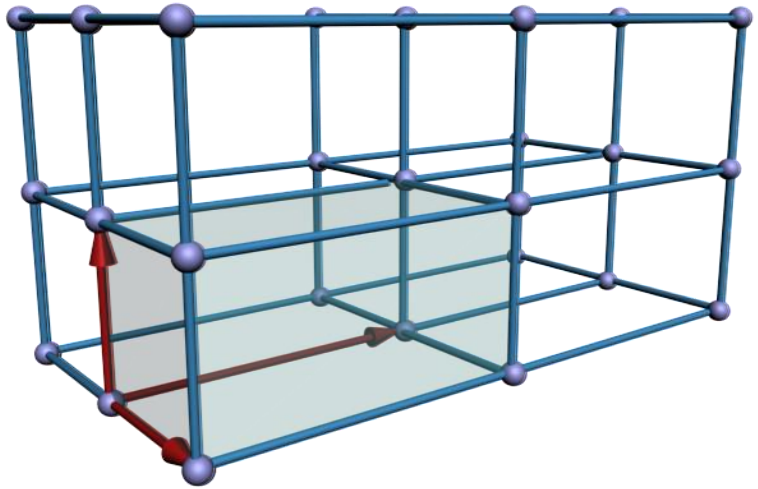
Primitive Cell for 3D Crystals

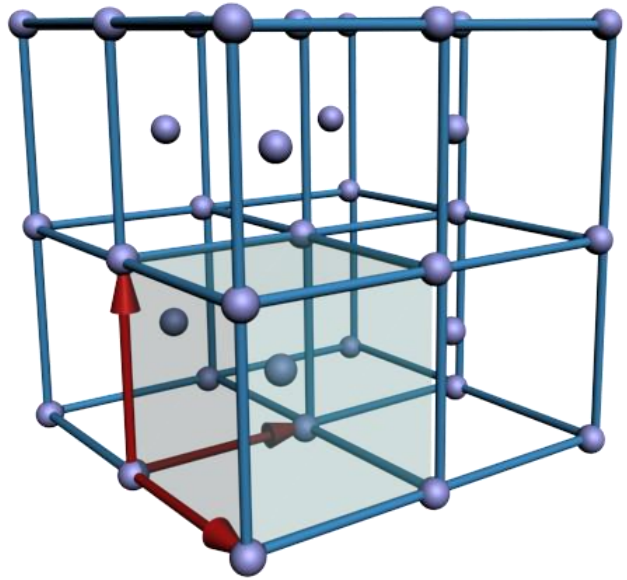
Standard model

- volume associated with one lattice point
- Parallelepiped with lattice points in the corner
- Each lattice point shared among 8 cells
- Number of lattice point/cell=8x1/8=1
- Vc= $|\mathbf{a}_1.(\mathbf{a}_2 x \mathbf{a}_3)|$

Crystallographic unit cell

- larger cell used to display the symmetries of the crystal
- Primitive





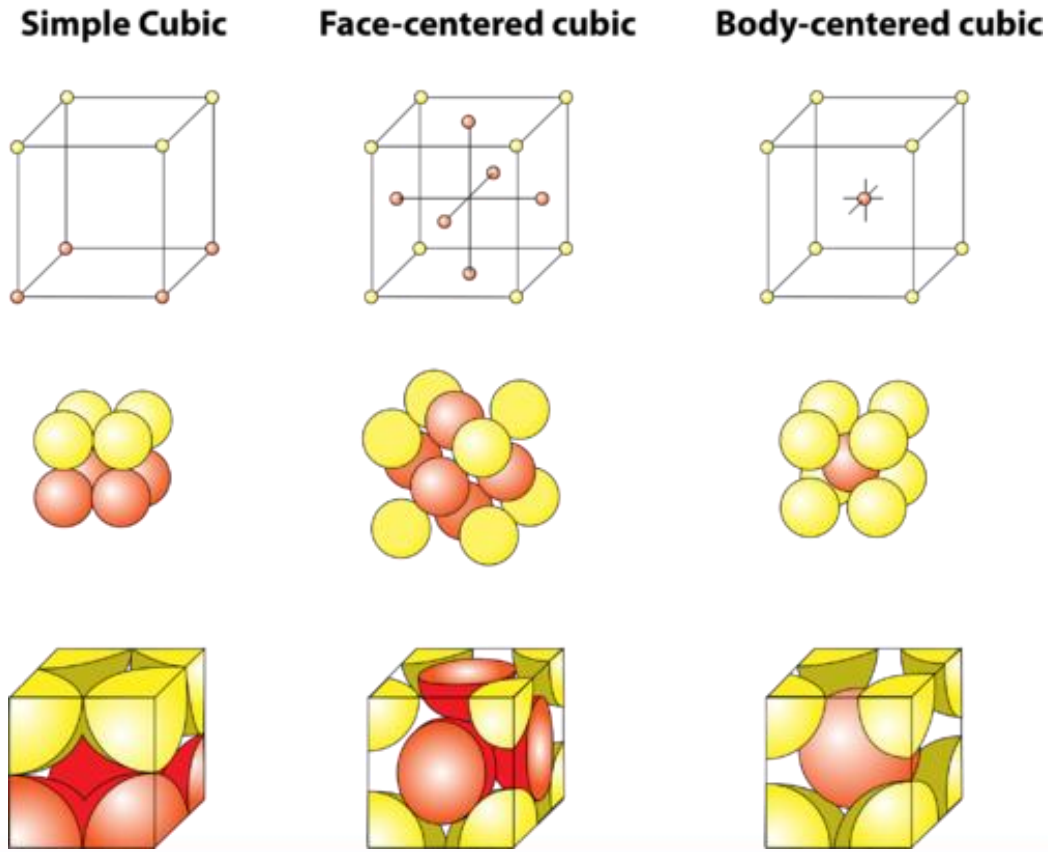
Not primitive

Bravais lattices in 3D

In 3D, there are 14 Bravais lattices. These are obtained by combining one of the 7 LATTICE SYSTEM with one of the centering types.

The centering types identify the locations of the lattice points in the unit cell as follows:

- **Primitive (P)**: lattice points on the cell corners only (~simple)
- Body-centered (I): lattice points on the cell corners, with one additional point at the center of the cell
- Face-centered (F): lattice points on the cell corners, with one additional point at the center of each of the faces of the cell
- Base-centered : lattice points on the cell corners with one additional point at the center of each face of one pair of parallel faces of the cell (sometimes called end-centered)

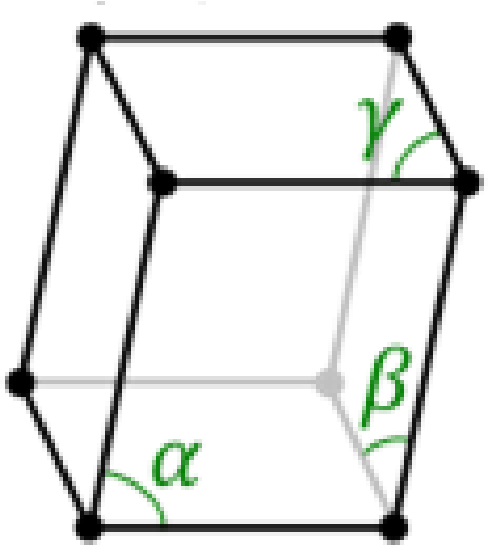


Crystal Family: Triclinic

In the triclinic system, the crystal is described by vectors of unequal length, as in the orthorhombic system. In addition, the angles between these vectors must all be different and may not include 90°.

System	Number of lattices	Cell axes and angles
Triclinic	**1**	**$\|a_1\| \neq \|a_2\| \neq \|a_3\|$, $\alpha \neq \beta \neq \gamma$**
Monoclinic	2	$\|a_1\| \neq \|a_2\| \neq \|a_3\|$, $\alpha = \gamma = 90° \neq \beta$
Orthorhombic	4	$\|a_1\| \neq \|a_2\| \neq \|a_3\|$, $\alpha = \beta = \gamma = 90°$
Tetragonal	2	$\|a_1\| = \|a_2\| \neq \|a_3\|$, $\alpha = \beta = \gamma = 90°$
Cubic	3	$\|a_1\| = \|a_2\| = \|a_3\|$, $\alpha = \beta = \gamma = 90°$
Trigonal	1	$\|a_1\| = \|a_2\| = \|a_3\|$, $\alpha = \beta = \gamma < 120° \neq 90°$
Hexagonal	1	$\|a_1\| = \|a_2\| \neq \|a_3\|$, $\alpha = \beta = 90°$ $\gamma = 120°$

An example of the triclinic crystals, microcline

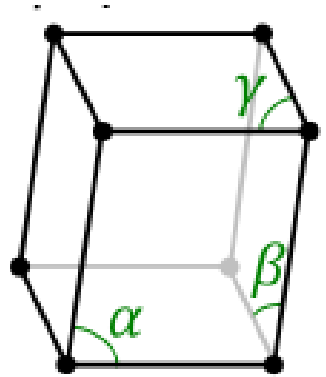


Monoclinic crystal system

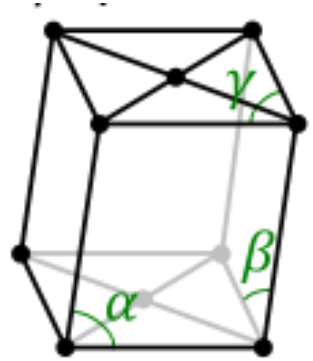
In the monoclinic system, the crystal is described by vectors of unequal lengths, as in the orthorhombic system. They form a rectangular prism with a parallelogram as its base. Hence two pairs of vectors are perpendicular, while the third pair makes an angle other than 90°.

An example of the monoclinic crystal orthoclase

system	Number of lattices	Cell axes and angles
Triclinic	1	$\|a_1\|\neq\|a_2\|\neq\|a_3\|$, $\alpha\neq\beta\neq\gamma$
Monoclinic	**2**	**$\|a_1\|\neq\|a_2\|\neq\|a_3\|$, $\alpha=\gamma=90°\neq\beta$**
Orthorhombic	4	$\|a_1\|\neq\|a_2\|\neq\|a_3\|$, $\alpha=\beta=\gamma=90°$
Tetragonal	2	$\|a_1\|=\|a_2\|\neq\|a_3\|$, $\alpha=\beta=\gamma=90°$
Cubic	3	$\|a_1\|=\|a_2\|=\|a_3\|$, $\alpha=\beta=\gamma=90°$
Trigonal	1	$\|a_1\|=\|a_2\|=\|a_3\|$, $\alpha=\beta=\gamma<120°\neq90°$
Hexagonal	1	$\|a_1\|=\|a_2\|\neq\|a_3\|$, $\alpha=\beta=90°$ $\gamma=120°$



Primitive monoclinic



Base centered monoclinic

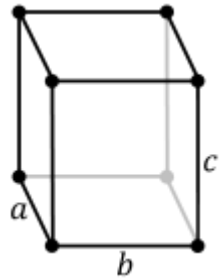
Orthorhombic crystal system

Orthorhombic lattices result from stretching a cubic lattice along two of its orthogonal pairs by two different factors, resulting in a rectangular prism with a rectangular base (*a* by *b*) and height (*c*), such that *a*, *b*, and *c* are distinct. All three bases intersect at 90° angles, so the three lattice vectors remain mutually orthogonal.

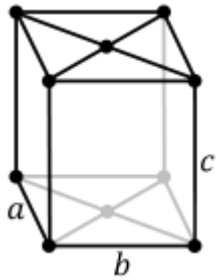
Hemimorphite

$Zn_4Si_2O_7(OH)_2 \cdot H_2O$

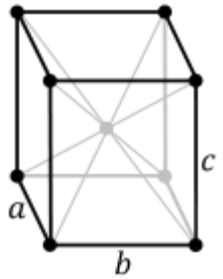
system	Number of lattices	Cell axes and angles
Triclinic	1	$\|a_1\| \neq \|a_2\| \neq \|a_3\|$, $\alpha \neq \beta \neq \gamma$
Monoclinic	2	$\|a_1\| \neq \|a_2\| \neq \|a_3\|$, $\alpha = \gamma = 90° \neq \beta$
Orthorhombic	**4**	**$\|a_1\| \neq \|a_2\| \neq \|a_3\|$, $\alpha = \beta = \gamma = 90°$**
Tetragonal	2	$\|a_1\| = \|a_2\| \neq \|a_3\|$, $\alpha = \beta = \gamma = 90°$
Cubic	3	$\|a_1\| = \|a_2\| = \|a_3\|$, $\alpha = \beta = \gamma = 90°$
Trigonal	1	$\|a_1\| = \|a_2\| = \|a_3\|$, $\alpha = \beta = \gamma < 120° \neq 90°$
Hexagonal	1	$\|a_1\| = \|a_2\| \neq \|a_3\|$, $\alpha = \beta = 90°$ $\gamma = 120°$



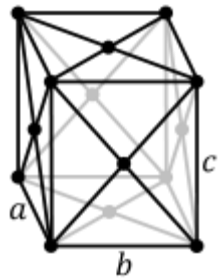
Primitive



Base centered orthorhombic



Body centered orthorhombic



Face centered orthorhombic

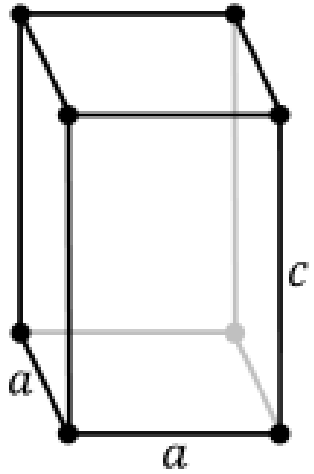
Tetragonal crystal system

Tetragonal crystal lattices result from stretching a cubic lattice along one of its lattice vectors, so that the cube becomes a rectangular prism with a square base (*a* by *a*) and height (*c*, which is different from *a*).

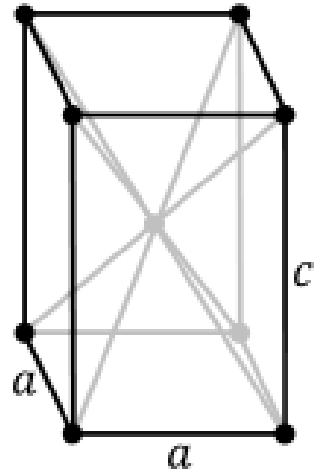
system	Number of lattices	Cell axes and angles
Triclinic	1	$\|a_1\|\neq\|a_2\|\neq\|a_3\|$, $\alpha\neq\beta\neq\gamma$
Monoclinic	2	$\|a_1\|\neq\|a_2\|\neq\|a_3\|$, $\alpha=\gamma=90°\neq\beta$
Orthorhombic	4	$\|a_1\|\neq\|a_2\|\neq\|a_3\|$, $\alpha=\beta=\gamma=90°$
Tetragonal	**2**	**$\|a_1\|=\|a_2\|\neq\|a_3\|$, $\alpha=\beta=\gamma=90°$**
Cubic	3	$\|a_1\|=\|a_2\|=\|a_3\|$, $\alpha=\beta=\gamma=90°$
Trigonal	1	$\|a_1\|=\|a_2\|=\|a_3\|$, $\alpha=\beta=\gamma<120°\neq90°$
Hexagonal	1	$\|a_1\|=\|a_2\|\neq\|a_3\|$, $\alpha=\beta=90°$ $\gamma=120°$

An example of the tetragonal crystals wulfenite $PbMoO_4$

Molybdate mineral



Primitive tetragonal



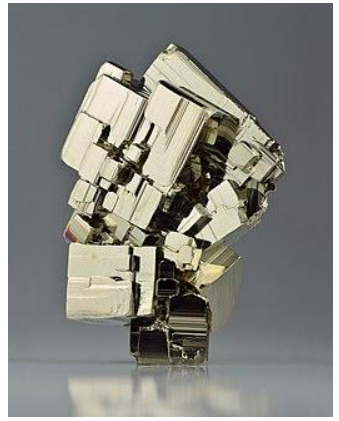
Body centered tetragonal

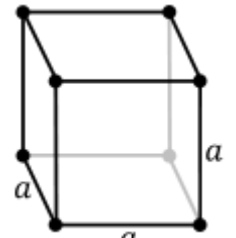
Cubic crystal system

This is one of the most common and simplest shapes found in crystals and minerals.

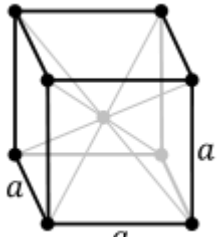
system	Number of lattices	Cell axes and angles
Triclinic	1	$\|a_1\| \neq \|a_2\| \neq \|a_3\|$, $\alpha \neq \beta \neq \gamma$
Monoclinic	2	$\|a_1\| \neq \|a_2\| \neq \|a_3\|$, $\alpha = \gamma = 90° \neq \beta$
Orthorhombic	4	$\|a_1\| \neq \|a_2\| \neq \|a_3\|$, $\alpha = \beta = \gamma = 90°$
Tetragonal	2	$\|a_1\| = \|a_2\| \neq \|a_3\|$, $\alpha = \beta = \gamma = 90°$
Cubic	**3**	**$\|a_1\| = \|a_2\| = \|a_3\|$, $\alpha = \beta = \gamma = 90°$**
Trigonal	1	$\|a_1\| = \|a_2\| = \|a_3\|$, $\alpha = \beta = \gamma < 120° \neq 90°$
Hexagonal	1	$\|a_1\| = \|a_2\| \neq \|a_3\|$, $\alpha = \beta = 90°$ $\gamma = 120°$

A rock containing three crystals of pyrite (FeS_2).

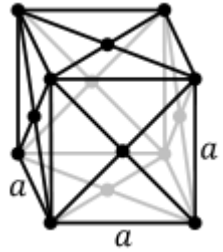




Simple cubic **sc**



Body centered cubic **bcc**



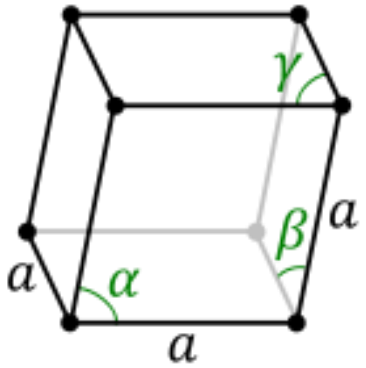
Face centered cubic **fcc**

Trigonal Crystal System

system	Number of lattices	Cell axes and angles
Triclinic	1	$\|a_1\| \neq \|a_2\| \neq \|a_3\|$, $\alpha \neq \beta \neq \gamma$
Monoclinic	2	$\|a_1\| \neq \|a_2\| \neq \|a_3\|$, $\alpha = \gamma = 90° \neq \beta$
Orthorhombic	4	$\|a_1\| \neq \|a_2\| \neq \|a_3\|$, $\alpha = \beta = \gamma = 90°$
Tetragonal	2	$\|a_1\| = \|a_2\| \neq \|a_3\|$, $\alpha = \beta = \gamma = 90°$
Cubic	3	$\|a_1\| = \|a_2\| = \|a_3\|$, $\alpha = \beta = \gamma = 90°$
Trigonal/ Rhombohedral	**1**	**$\|a_1\| = \|a_2\| = \|a_3\|$, $\alpha = \beta = \gamma < 120° \neq 90°$**
Hexagonal	1	$\|a_1\| = \|a_2\| \neq \|a_3\|$, $\alpha = \beta = 90°$ $\gamma = 120°$

Carbonate minerals

Dolomite (white) on talc



The **hexagonal crystal family** is one of the six crystal families, which includes two crystal systems (hexagonal and **trigonal**) and two lattice systems (hexagonal and **trigonal/rhombohedral**)

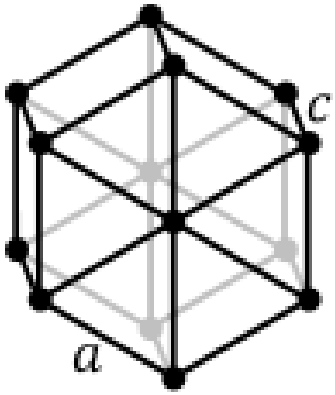
Hexagonal crystal system

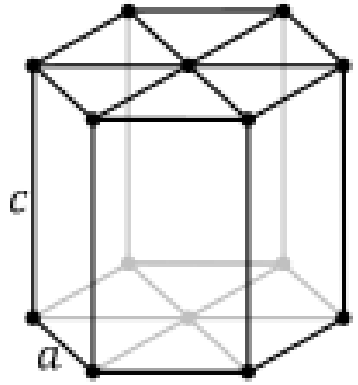
Hexagonal close packed (hcp) is one of the two simple types of atomic packing with the highest density

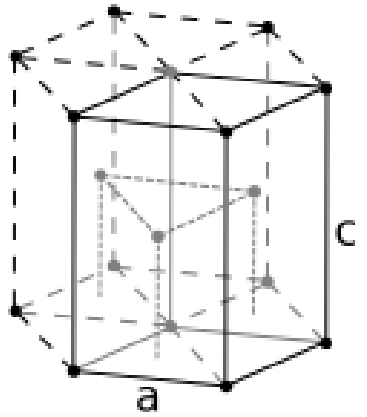
system	Number of lattices	Cell axes and angles
Triclinic	1	$\|a_1\|\neq\|a_2\|\neq\|a_3\|$, $\alpha\neq\beta\neq\gamma$
Monoclinic	2	$\|a_1\|\neq\|a_2\|\neq\|a_3\|$, $\alpha=\gamma=90°\neq\beta$
Orthorhombic	4	$\|a_1\|\neq\|a_2\|\neq\|a_3\|$, $\alpha=\beta=\gamma=90°$
Tetragonal	2	$\|a_1\|=\|a_2\|\neq\|a_3\|$, $\alpha=\beta=\gamma=90°$
Cubic	3	$\|a_1\|=\|a_2\|=\|a_3\|$, $\alpha=\beta=\gamma=90°$
Trigonal	1	$\|a_1\|=\|a_2\|=\|a_3\|$, $\alpha=\beta=\gamma<120°\neq90°$
Hexagonal	**1**	**$\|a_1\|=\|a_2\|\neq\|a_3\|$, $\alpha=\beta=90°$ $\gamma=120°$**

α-Quartz

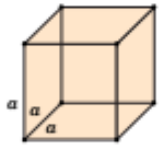
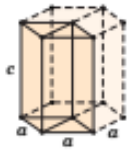
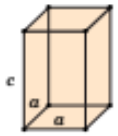
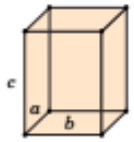
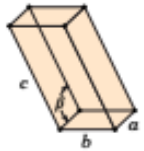
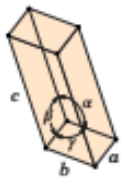
Beryl/ Cyclosilicate



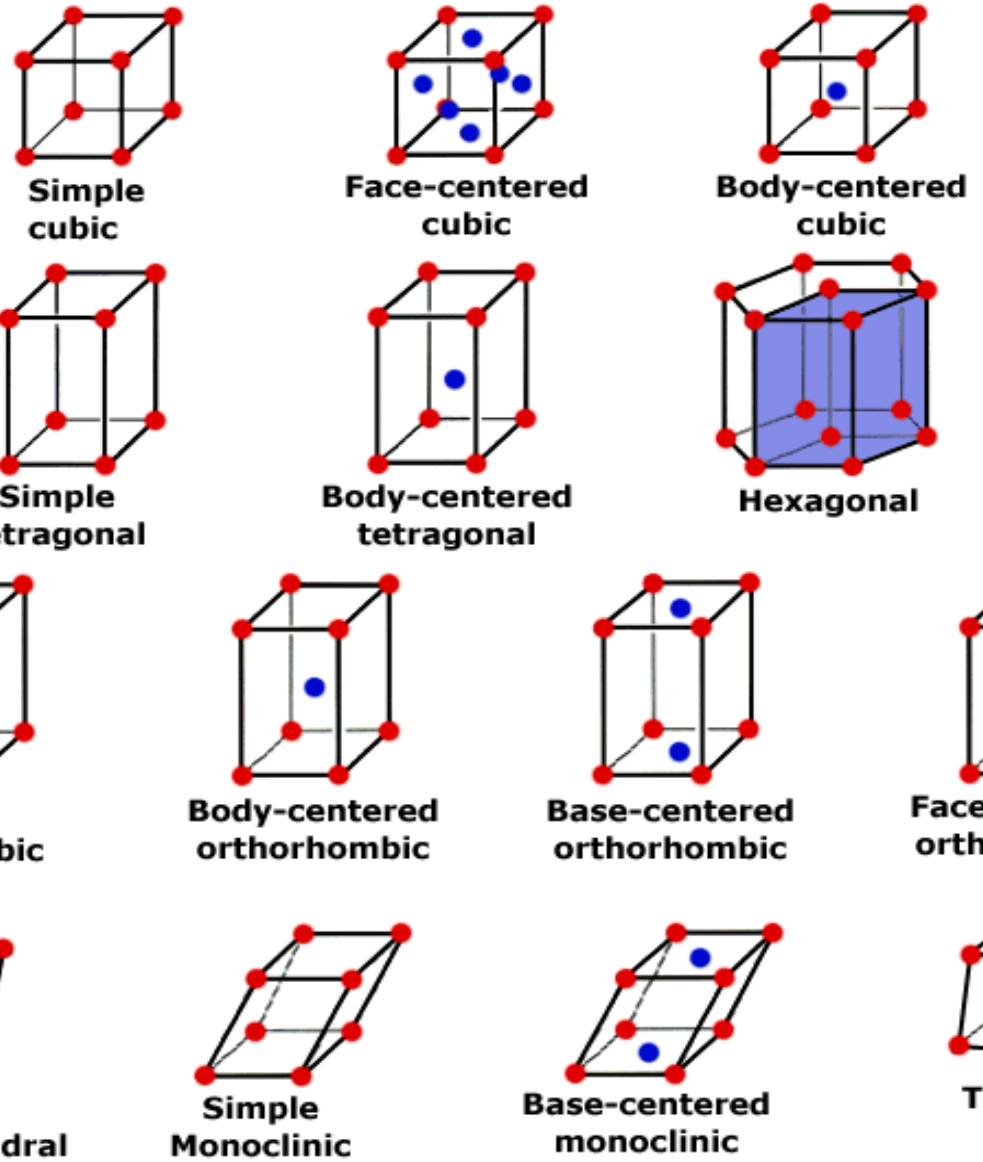




Bravais Lattice

Crystal System	Axial Relationships	Interaxial Angles	Unit Cell Geometry
Cubic	$a = b = c$	$\alpha = \beta = \gamma = 90°$	
Hexagonal	$a = b \neq c$	$\alpha = \beta = 90°, \gamma = 120°$	
Tetragonal	$a = b \neq c$	$\alpha = \beta = \gamma = 90°$	
Rhombohedral (Trigonal)	$a = b = c$	$\alpha = \beta = \gamma \neq 90°$	
Orthorhombic	$a \neq b \neq c$	$\alpha = \beta = \gamma = 90°$	
Monoclinic	$a \neq b \neq c$	$\alpha = \gamma = 90° \neq \beta$	
Triclinic	$a \neq b \neq c$	$\alpha \neq \beta \neq \gamma \neq 90°$	

14 types of unit cells under seven crystal systems



14 Bravais Lattices divided into 7 Crystal Systems

	Crystal System	Shape of UC	Bravais Lattices			
			P	I	F	C
1	Cubic	Cube	✓	✓	✓	
2	Tetragonal	Square Prism (general height)	✓	✓		
3	Orthorhombic	Rectangular Prism (general height)	✓	✓	✓	✓
4	Hexagonal	120° Rhombic Prism	✓			
5	Trigonal	Parallopiped (Equilateral, Equiangular)	✓			
6	Monoclinic	Parallogramic Prism	✓			✓
7	Triclinic	Parallopiped (general)	✓			

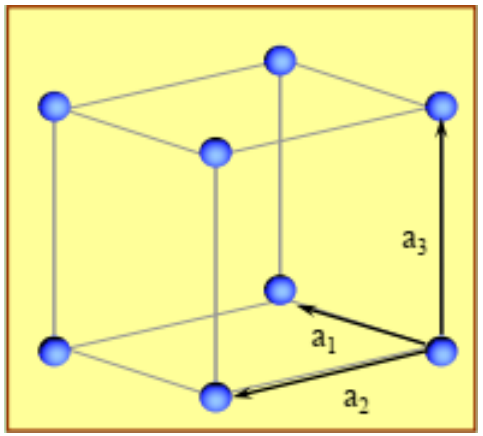
P	Primitive
I	Body Centred
F	Face Centred
C	Base- Centred

Metallic Crystal Structures

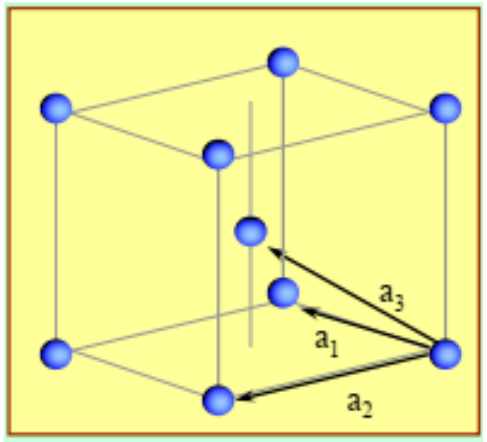
- Metals are usually (poly)crystalline; although formation of amorphous metals is possible by rapid cooling
- The atomic bonding in metals is non-directional ⇒ no restriction on numbers or positions of nearest-neighbor atoms ⇒ large number of nearest neighbors and dense atomic packing

- **The most common types of unit cells are**
  - faced-centered cubic (FCC)
  - body-centered cubic (BCC)
  - hexagonal close-packed (HCP)

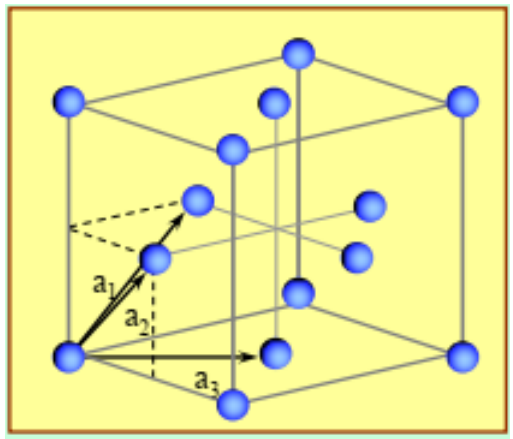
Atomic packing factor, APF = fraction of volume occupied by hard spheres



Simple Cubic lattice



Body-Centred Cubic lattice



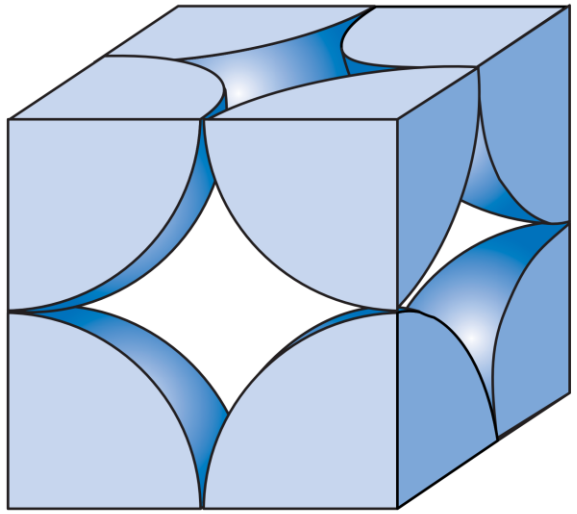
Face-Centred Cubic lattice

$$\text{APF} = \frac{\text{Sum of atomic volumes}}{\text{Volume of cell}}$$

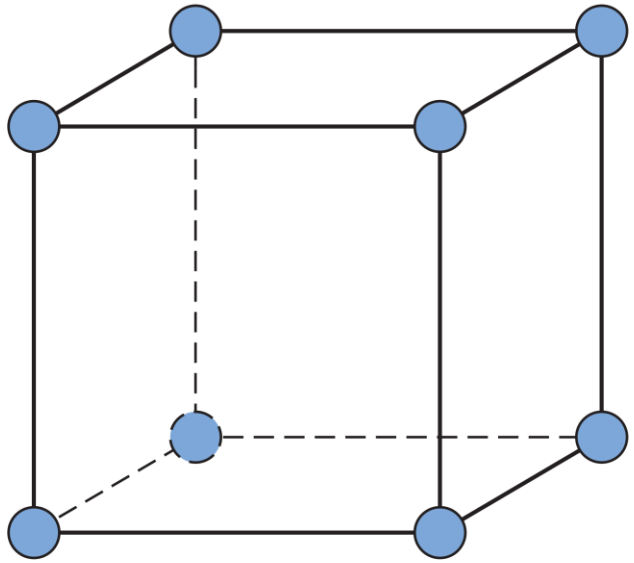
Number of Atoms per Unit Cell, N,

$$N = N_i + \frac{N_f}{2} + \frac{N_c}{8}$$

Simple cubic (SC) crystal structure



(a)



(b)

For the simple cubic crystal structure,
(*a*) a hard-sphere unit cell, and (*b*) a reduced-sphere unit cell.

Number of Atoms per Unit Cell, N,

$$N = N_i + \frac{N_f}{2} + \frac{N_c}{8} \longrightarrow N = 0 + 0 + 8/8 = 1$$

(Primitive Unit cell)

$$\text{APF} = \frac{\text{Sum of atomic volumes}}{\text{Volume of cell}}$$

$$\text{APF} = \frac{N_{\text{atoms}} V_{\text{atom}}}{V_{\text{unit cell}}} = \frac{1 \cdot \frac{4}{3}\pi r^3}{(2r)^3}$$

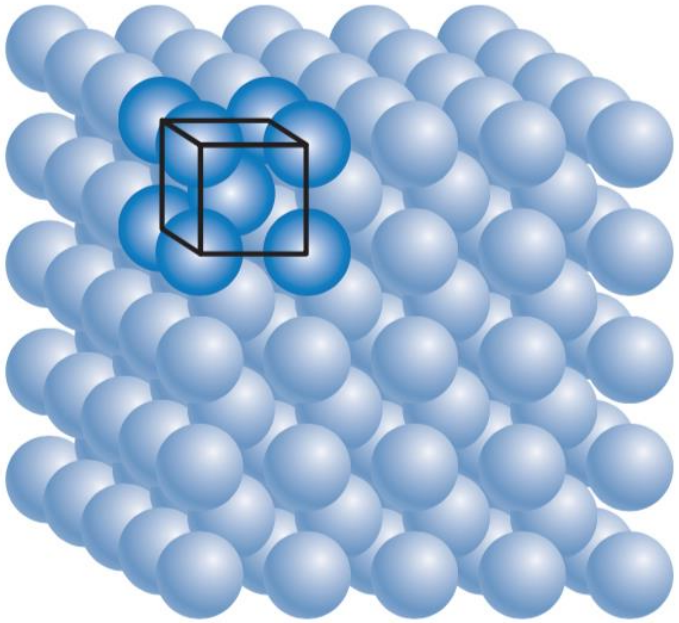
$$= \frac{\pi}{6} \approx 0.5236$$

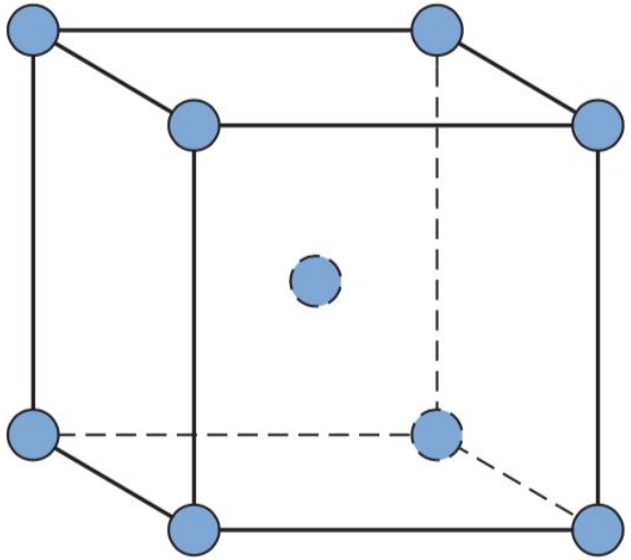
APF : 0.52

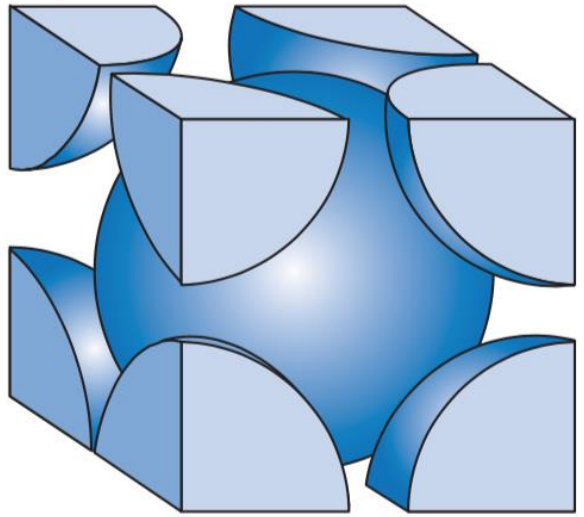
- None of the metallic elements have this crystal structure because of its relatively low atomic packing factor.
- The **only simple-cubic element is polonium**, which is considered to be a metalloid (or semi-metal).

Body - centered cubic structure

Atom at each corner and at center of cubic unit cell : Cr, α-Fe, Mo, W have this crystal structure







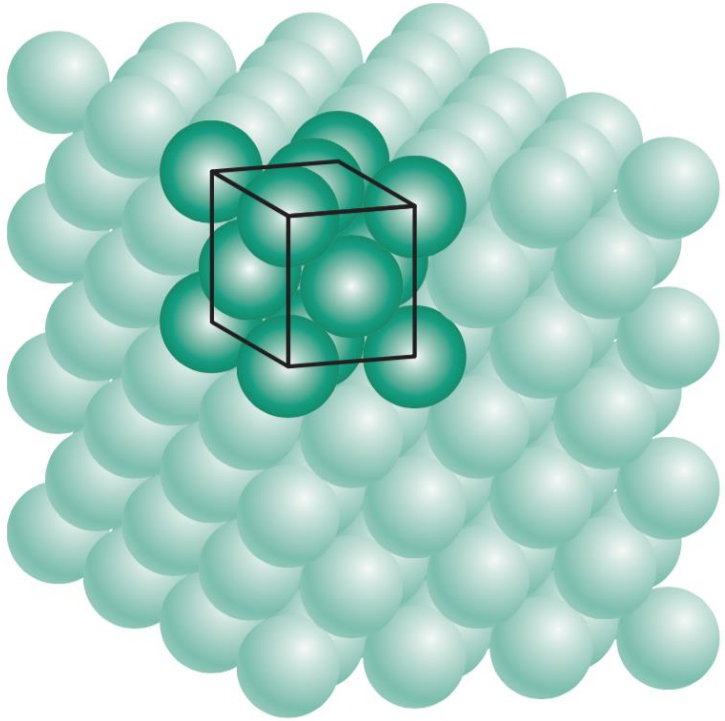
- The hard spheres touch one another along cube diagonal
  ⇒ **the cube edge length, a= 4R/√3**
- **The coordination number, CN = 8**
- **Number of atoms per unit cell, n = 2**
  Center atom (1) shared by no other cells: 1 x 1 = 1
  8 corner atoms shared by eight cells: 8 x 1/8 = 1
- **Atomic packing factor, APF = 0.68**

$$N = N_i + \frac{N_f}{2} + \frac{N_c}{8}$$

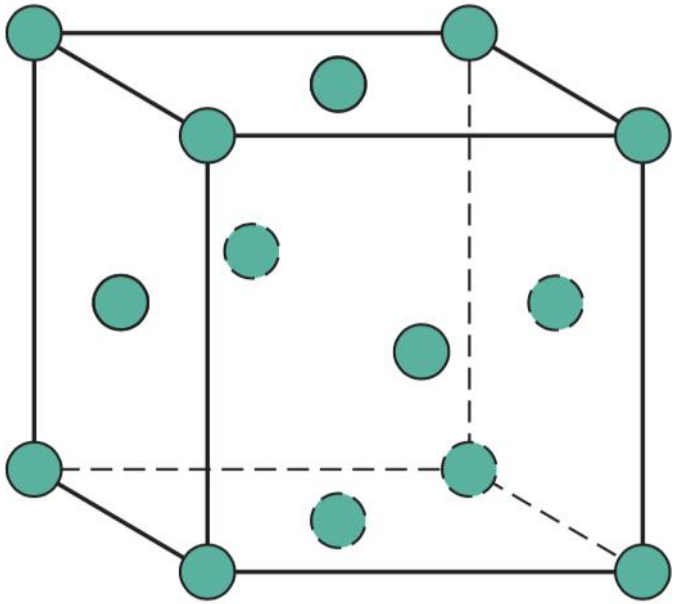
$$= 1 + 0 + \frac{8}{8} = 2$$

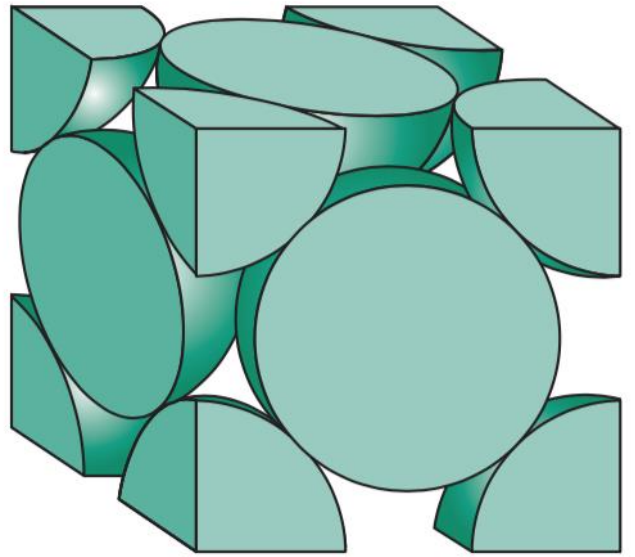
Face - Centered Cubic (FCC) Crystal Structure

- Atoms are located at each of the corners and on the centers of all the faces of cubic unit cell
- Cu, Al, Ag, Au have this crystal structure

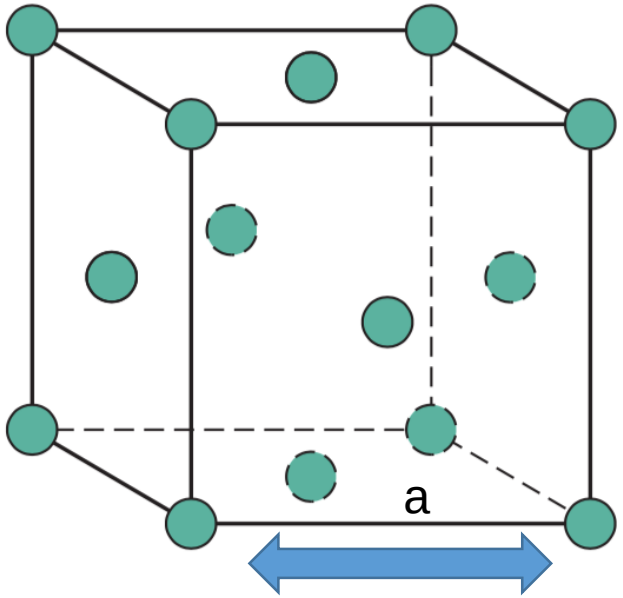


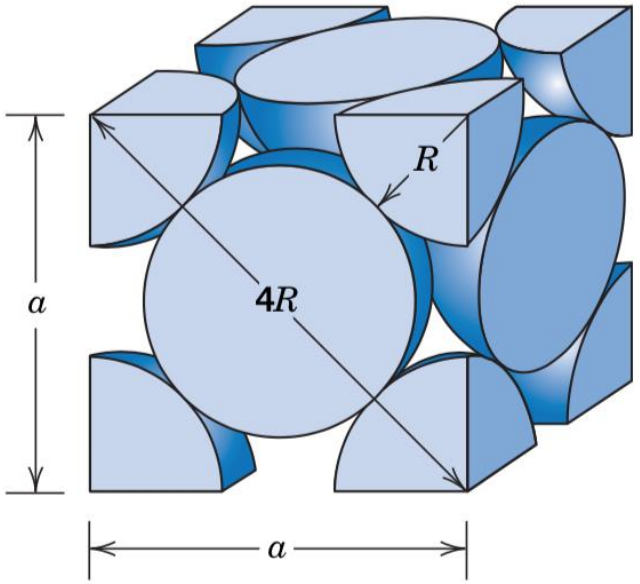
Two representations of the FCC unit cell





Face - Centered Cubic (FCC) Crystal Structure





Number of Atoms per Unit Cell, N,

$$N = N_i + \frac{N_f}{2} + \frac{N_c}{8}$$

$$N = 0 + \frac{6}{2} + \frac{8}{8} = 4$$

Number of atoms per unit cell, N = 4

The hard spheres touch one another across a face diagonal ⇒ the cube edge length, **a= 2R√2**

The coordination number, CN = the number of closest neighbors to which an atom is bonded = number of touching atoms, **CN = 12**

$$\textbf{APF} = \frac{\text{Sum of atomic volumes}}{\text{Volume of cell}}$$

Volume of 4 hard spheres in the unit cell: $4 \times \frac{4}{3}\pi R^3$

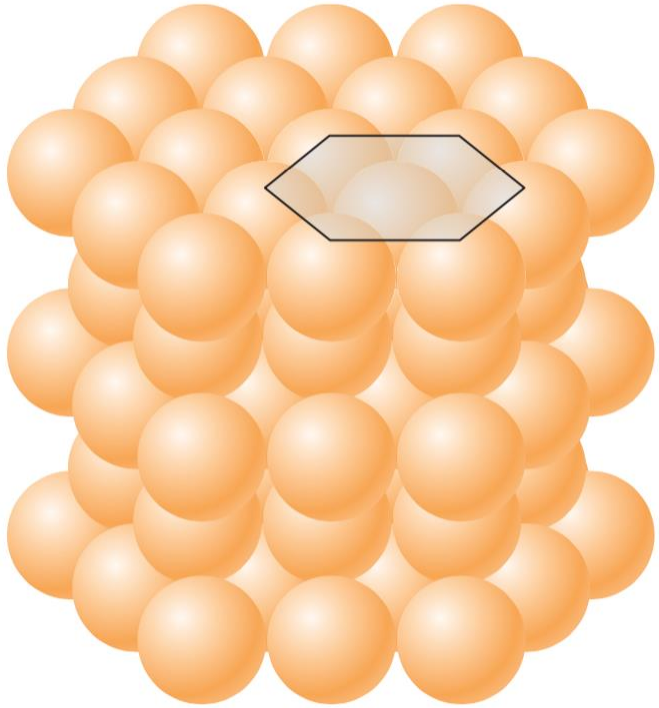
Volume of the unit cell: $a^3 = 16R^3\sqrt{2}$

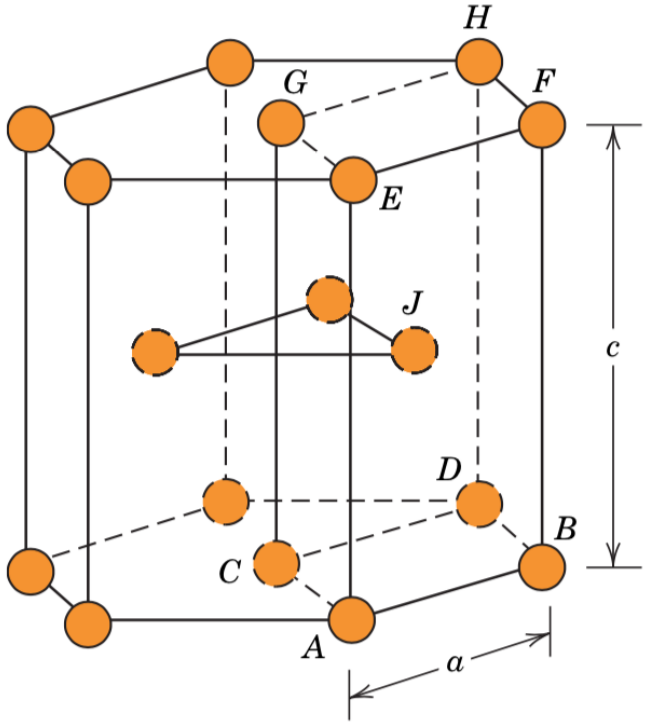
$$APF = \frac{16}{3}\pi R^3 \Big/ 16R^3\sqrt{2} = \pi/3\sqrt{2} = 0.74$$

maximum possible packing of hard spheres

Hexagonal close – packed 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
- Cd, Mg, Zn, Ti have this crystal structure





- **Number of atoms per unit cell,**
  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

$$N = N_i + \frac{N_f}{2} + \frac{N_c}{6}$$

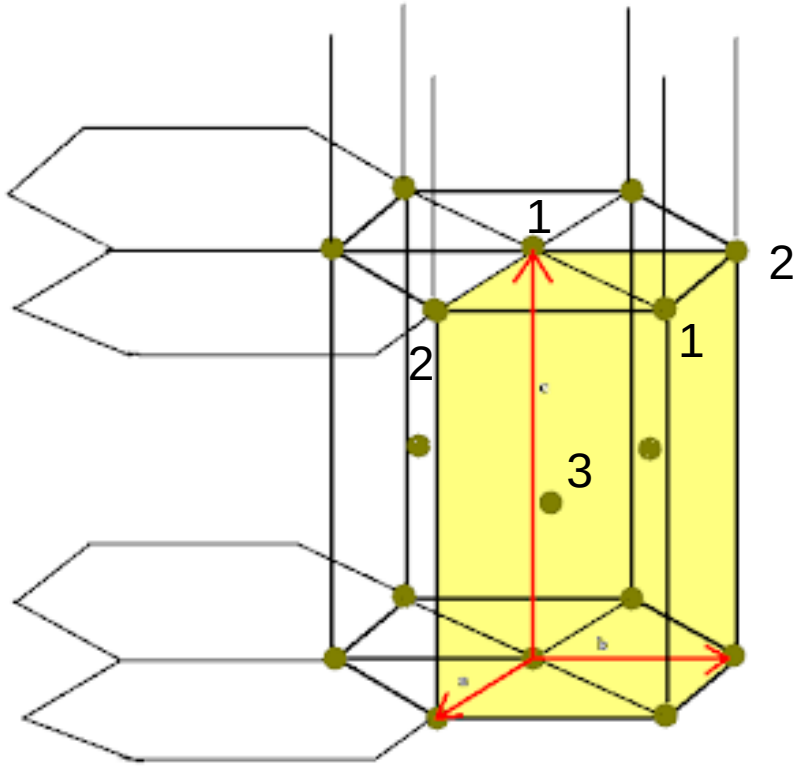
$$N = 3 + \frac{2}{2} + \frac{12}{6} = 6$$

The coordination number, CN = 12 (same as in FCC)

Atomic packing factor, APF = 0.74 (same as in FCC)

Isolated HCP Unit Cell

The isolated HCP unit cell also called the primitive cell?



Position 1 contributes = 1/6

Position 2 contributes = 1/12

Total Atom: 4 (1/6) + 4 (1/12) = 1

Position 3 contributes = 1

"3" centered inside the unit cell but extends beyond the boundary of the cell

Total Atom per unit cell : 4 (1/6) + 4 (1/12) + 1= 2

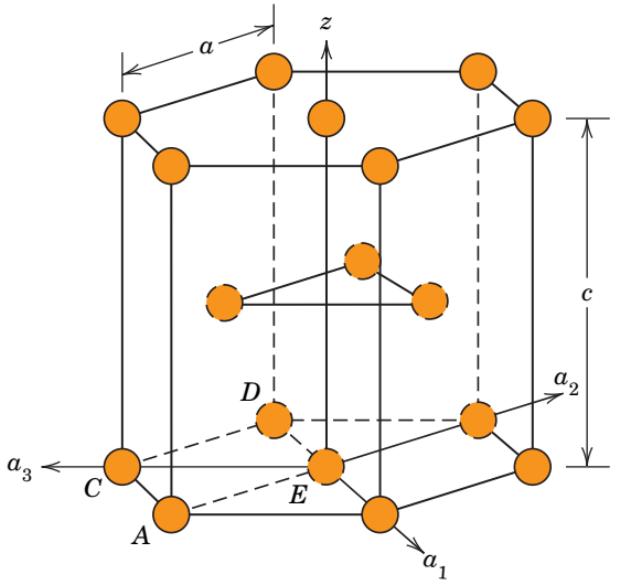
- The c/a ratio for an ideal HCP crystal structure consisting of uniform spheres packed as tightly together as possible is 1.633.

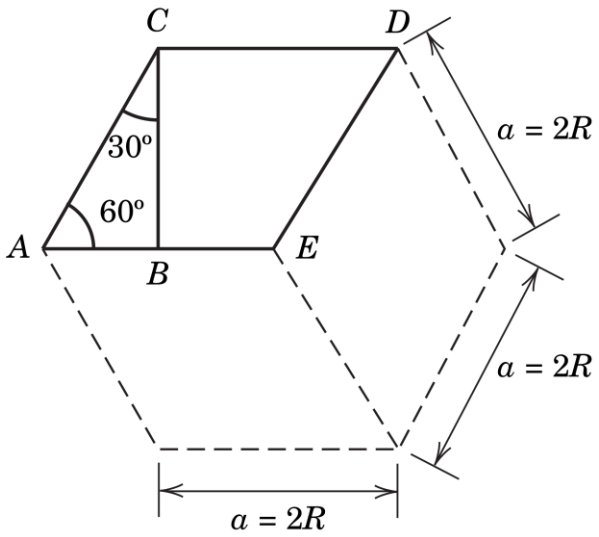
Metal	Lattice constants (nm) *a*	Lattice constants (nm) *c*	Atomic radius *R* (nm)	*c/a* ratio	% deviation from ideality
Cadmium	0.2973	0.5618	0.149	1.890	+15.7
Zinc	0.2665	0.4947	0.133	1.856	+13.6
Ideal HCP				1.633	0
Magnesium	0.3209	0.5209	0.160	1.623	−0.66
Cobalt	0.2507	0.4069	0.125	1.623	−0.66
Zirconium	0.3231	0.5148	0.160	1.593	−2.45
Titanium	0.2950	0.4683	0.147	1.587	−2.81
Beryllium	0.2286	0.3584	0.113	1.568	−3.98

Slightly elongated along c

Slightly compressed along c

Determination of HCP Unit Cell Volume





The unit cell volume is just the product of the base area times the cell height, *c*.

The area of $ACDE$ is just the length of $\overline{CD}$ times the height $\overline{BC}$. But $\overline{CD}$ is just a, and $\overline{BC}$ is equal to

$$\overline{BC} = a\cos(30°) = \frac{a\sqrt{3}}{2}$$

Thus, the base area is just

$$\text{AREA} = (3)(\overline{CD})(\overline{BC}) = (3)(a)\left(\frac{a\sqrt{3}}{2}\right) = \frac{3a^2\sqrt{3}}{2}$$

Again, the unit cell volume V_C is just the product of the AREA and c; thus,

$$V_C = \text{AREA}(c) = \left(\frac{3a^2\sqrt{3}}{2}\right)(c) = \frac{3a^2c\sqrt{3}}{2}$$

$$a = 2R$$

Now making this substitution for a in Equation 3.7a gives

$$V_C = \frac{3(2R)^2c\sqrt{3}}{2} = 6R^2c\sqrt{3}$$

Home work :

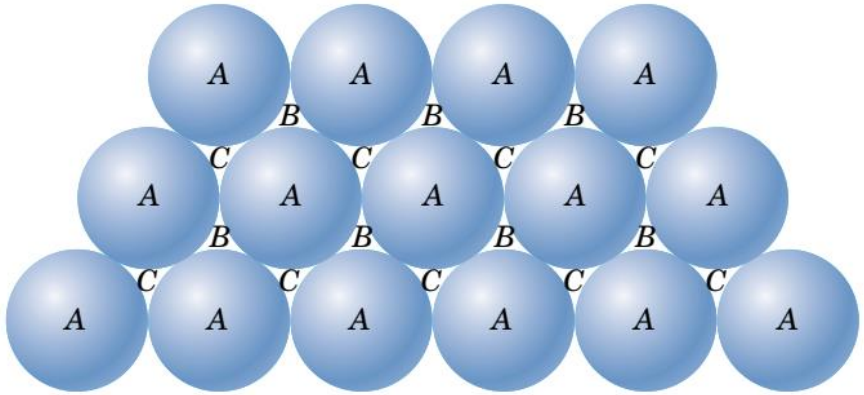
Unit cell has two lattice parameters a and c. Show the Ideal ratio **c/a = 1.633 ?**

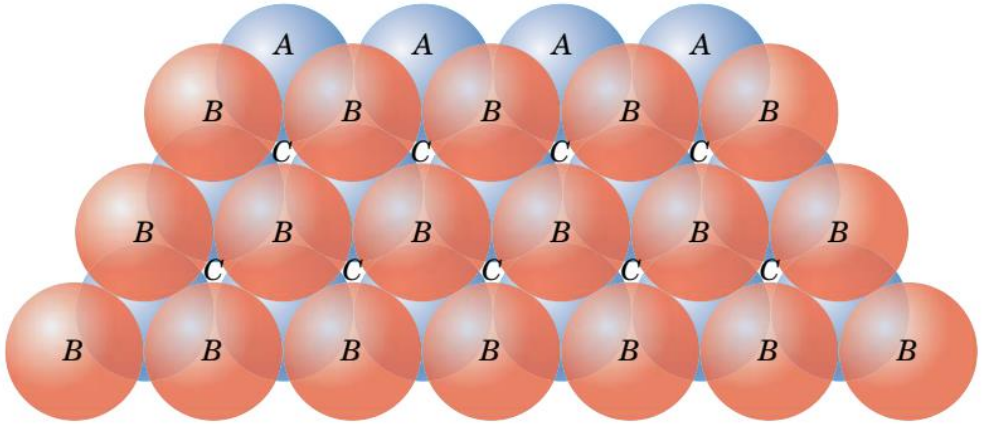
Atomic packing factor, APF = 0.74 (same as in FCC)

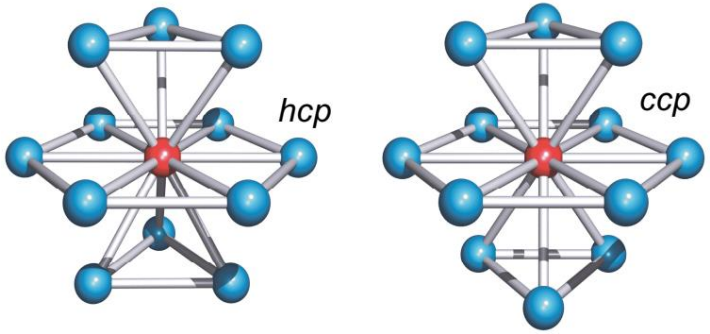
Close-packed Structures (FCC and HCP)

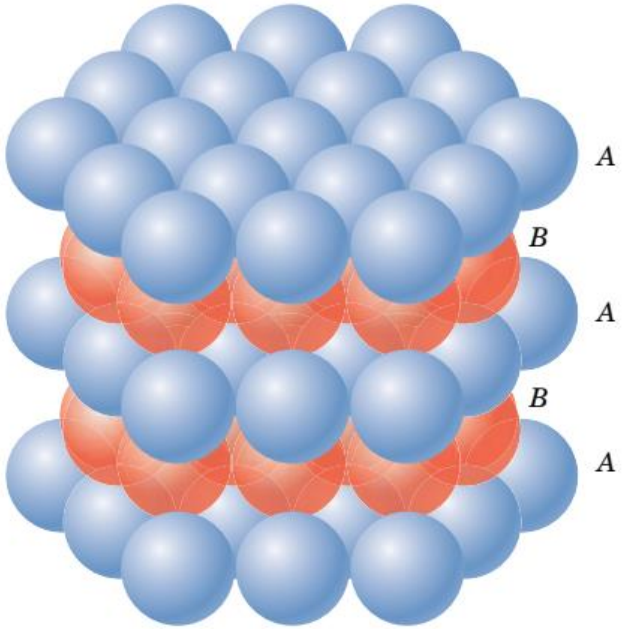
- Both FCC and HCP crystal structures have atomic packing factors of 0.74
- Both FCC and HCP crystal structures may be generated by the stacking of close-packed planes

The difference between the two structures is in the stacking sequence

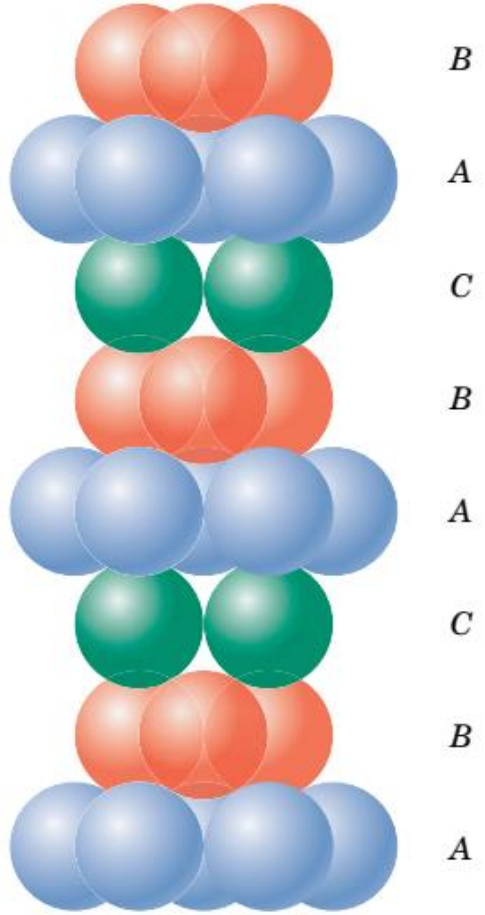








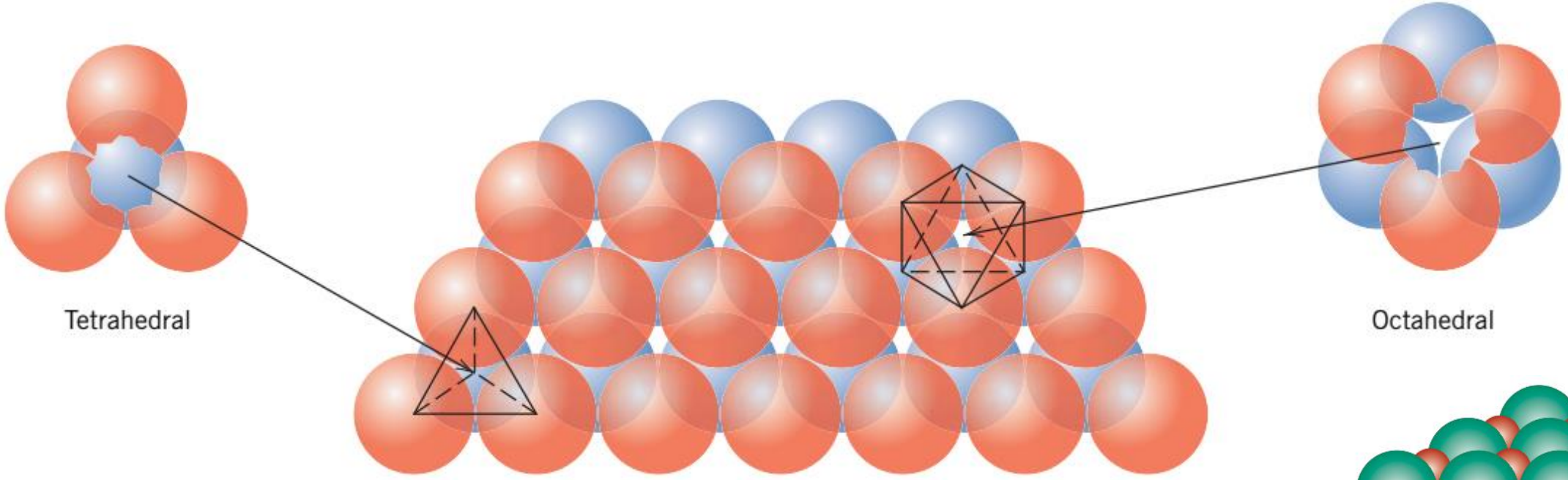
HCP: ABABAB...



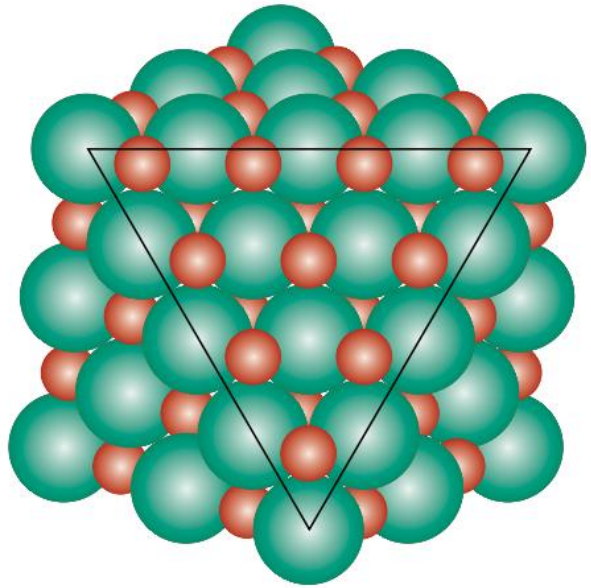
FCC: ABCABCABC…

Close-packed Structures: Tetrahedral ~ Octahedral

The stacking of one plane of close-packed (orange) spheres (anions) on top of another (blue spheres); the geometries of tetrahedral and octahedral positions between the planes are noted.

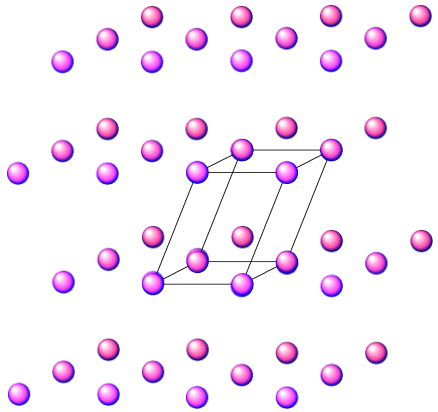


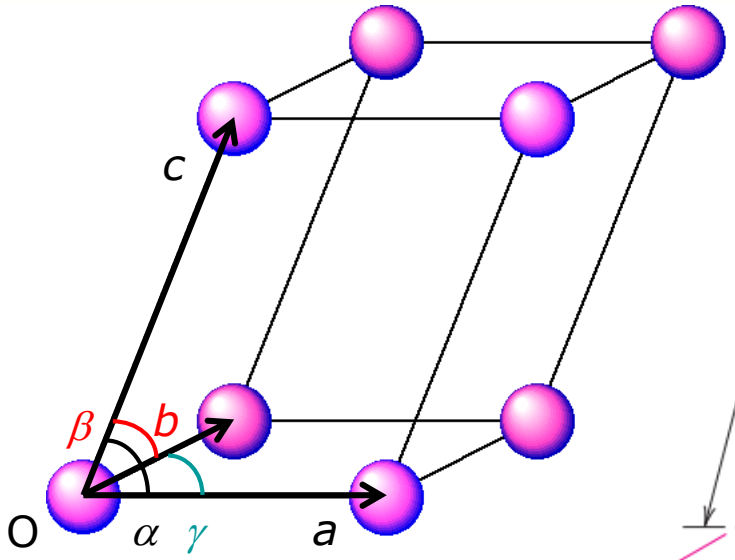
A section of the rock salt crystal structure from which a corner has been removed. The exposed plane of anions (green spheres inside the triangle) is a {111}-type plane; the cations (red spheres) occupy the interstitial octahedral positions.

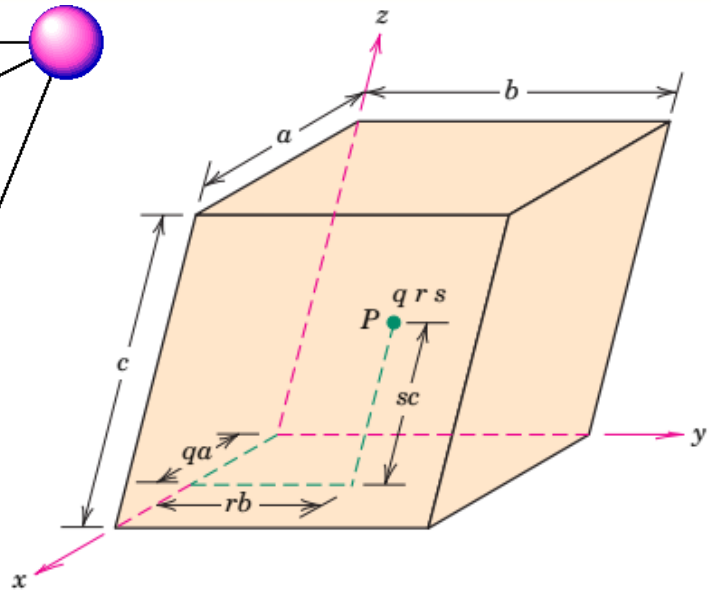


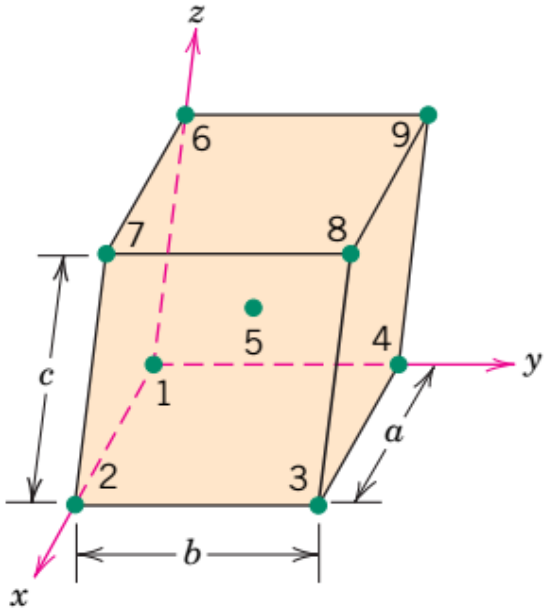
Unit Cell : **Point Coordinates**

Unit cell in a crystal :









a, *b* and *c* : crystal axes

|*a*|, |*b*|, |*c*|, α, β and γ : lattice constants

- **It is necessary to specify a lattice position using three *point coordinate indices: q*, *r*, and *s*.**
- **These indices are fractional multiples of *a*, *b*, and *c* unit cell edge lengths**

***a/q*, *b/r*, *c/s* : ratios → smallest integers**

***q*, *r* and *s* : coordinates ($\bar{u}$: negative)**

Point Number	*q*	*r*	*s*
1	0	0	0
2	1	0	0
3	1	1	0
4	0	1	0
5	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$
6	0	0	1
7	1	0	1
8	1	1	1
9	0	1	1

Directions in the Unit Cell

Crystallographic direction: a line directed between two points, or a *vector*.

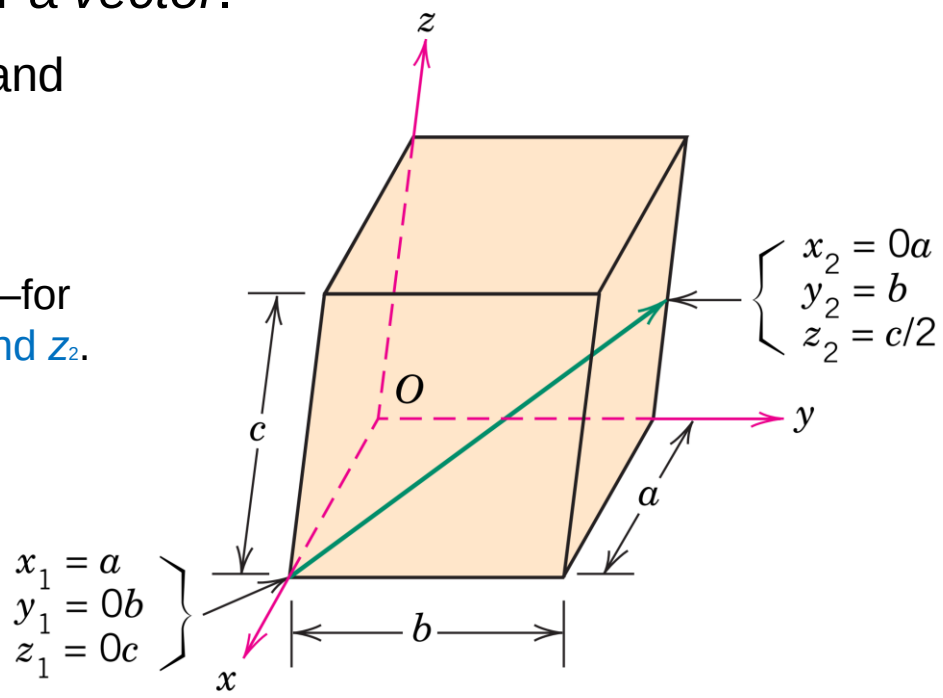
Miller-indices - notation to describe certain crystallographic directions and planes in a material

1. **First construct** *x-y-z* coordinate system
2. The coordinates of two points that lie on the direction vector are determined—for example, Point 1: x_1, y_1, and z_1; whereas for the vector head, Point 2: x_2, y_2, and z_2.
3. Tail point coordinates are subtracted from head point components—that is, $x_2 - x_1$, $y_2 - y_1$, and $z_2 - z_1$.
4. These coordinate differences are then normalized by *a*, *b*, and *c* lattice parameters

$$\frac{x_2 - x_1}{a} \quad \frac{y_2 - y_1}{b} \quad \frac{z_2 - z_1}{c}$$

5. Reduce them to the smallest integer values.

6. The three resulting **indices, [*uvw*]**. The *u*, *v*, and *w* integers correspond to the normalized coordinate differences referenced to the *x*, *y*, and *z* axes, respectively.



$$u = n\left(\frac{x_2 - x_1}{a}\right)$$

$$v = n\left(\frac{y_2 - y_1}{b}\right)$$

$$w = n\left(\frac{z_2 - z_1}{c}\right)$$

$$x_2 = ua + x_1$$

$$y_2 = vb + y_1$$

$$z_2 = wc + z_1$$

A direction in a unit cell

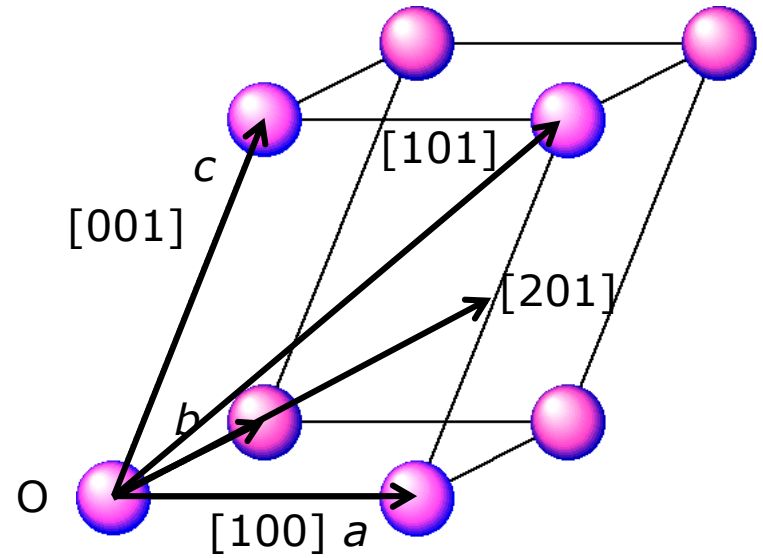
a, *b* and *c* : axes of coordinate/ lattice constants

***a/u*, *b/v*, *c/w* : ratios → smallest integers**

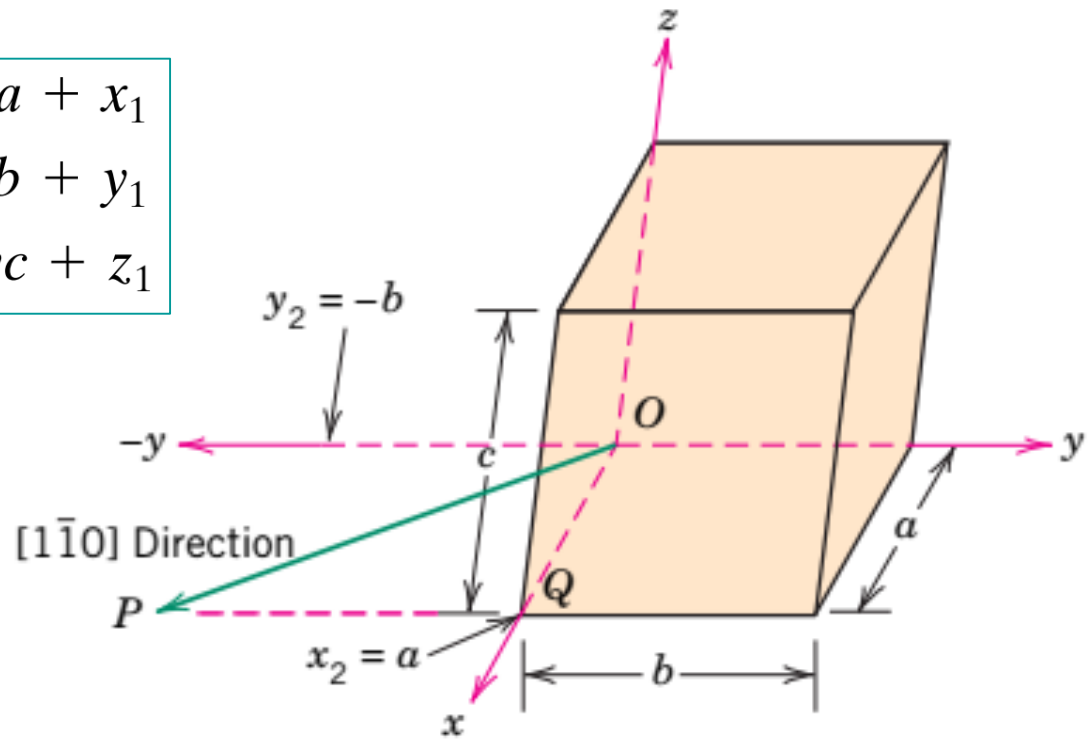
u, *v* and *w* : coordinates ($\bar{u}$: negative)

[*x y z*] : lattice directions

<*x y z*> : directions of a form <100> = [100], [010], [001], ...



$$x_2 = ua + x_1$$
$$y_2 = vb + y_1$$
$$z_2 = wc + z_1$$



Construction of a Specified Crystallographic Direction

Within the following unit cell draw a [1$\bar{1}$0] direction with its tail located at the origin of the coordinate system, point *O*.