

Periodicity and Solids

Crystals and Symmetry

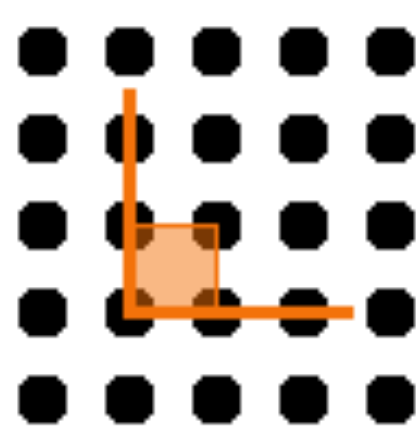
Definitions

- Lattice: A collection of points such that the surrounding arrangement will remain invariant.
- Lattice translational vectors: Set of vectors connecting two lattice points
- Lattice vectors: Basis vectors of the lattice translational vectors
- Total number of lattice vectors is the dimension of the system
- Motif: Collection of atoms at each lattice point.

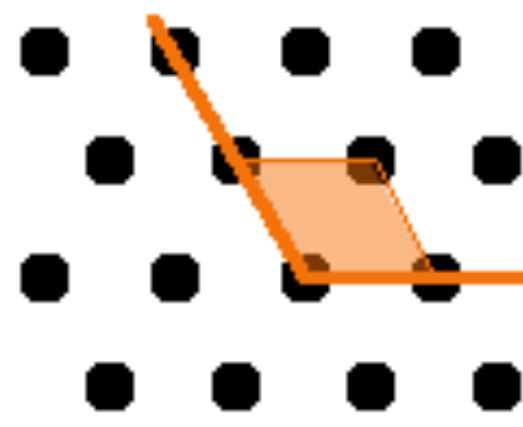
Definitions

- Primitive cell: Volume enclosed by the lattice vectors
- Unit cell: Convenient volume that can be repeated to obtain an infinite crystal

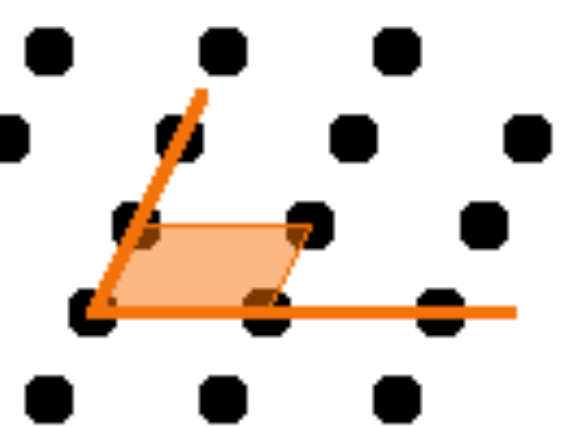
Bravais in 2D



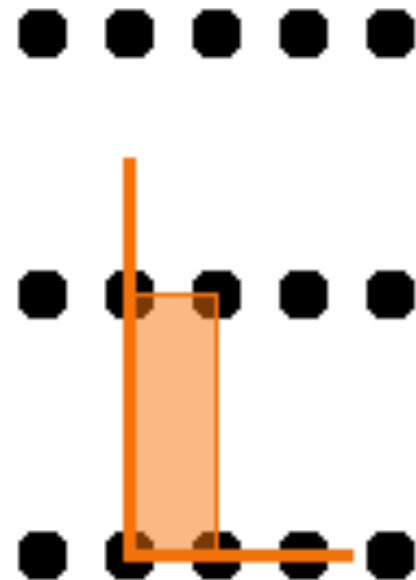
square
 $a = b \quad \gamma = 90^\circ$



hexagonal
 $a = b \quad \gamma = 120^\circ$

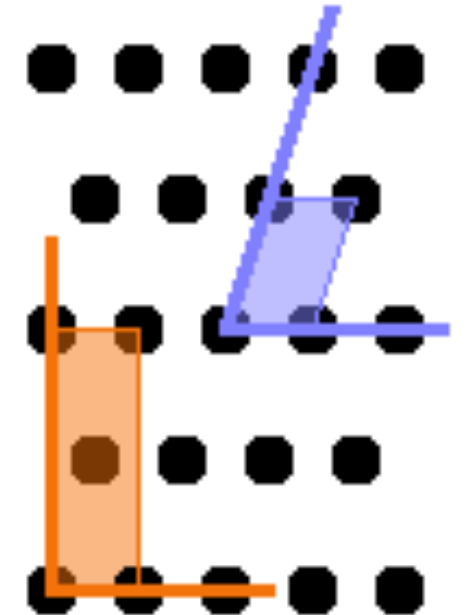


oblique
 $a \neq b \quad \gamma \neq 90^\circ$



**rectangular
primitive**

$a \neq b \quad \gamma = 90^\circ$

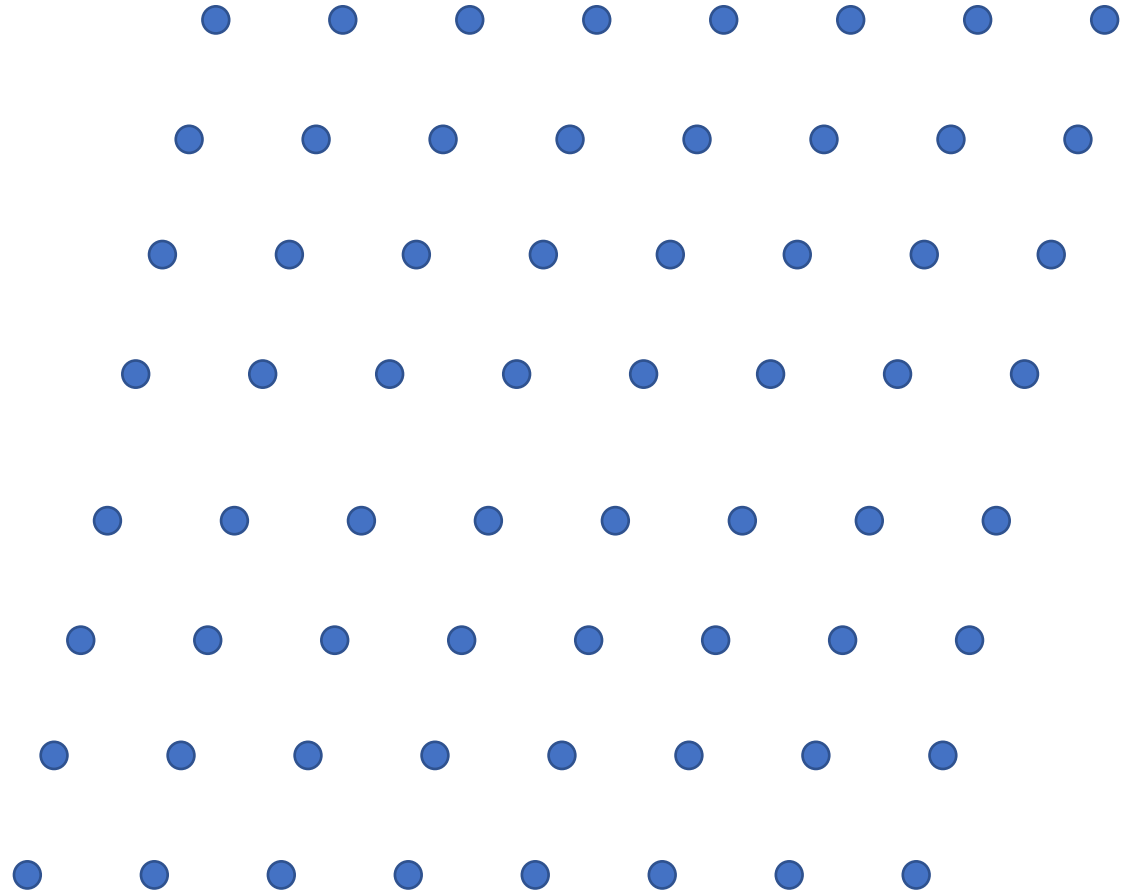


**rectangular
centred**

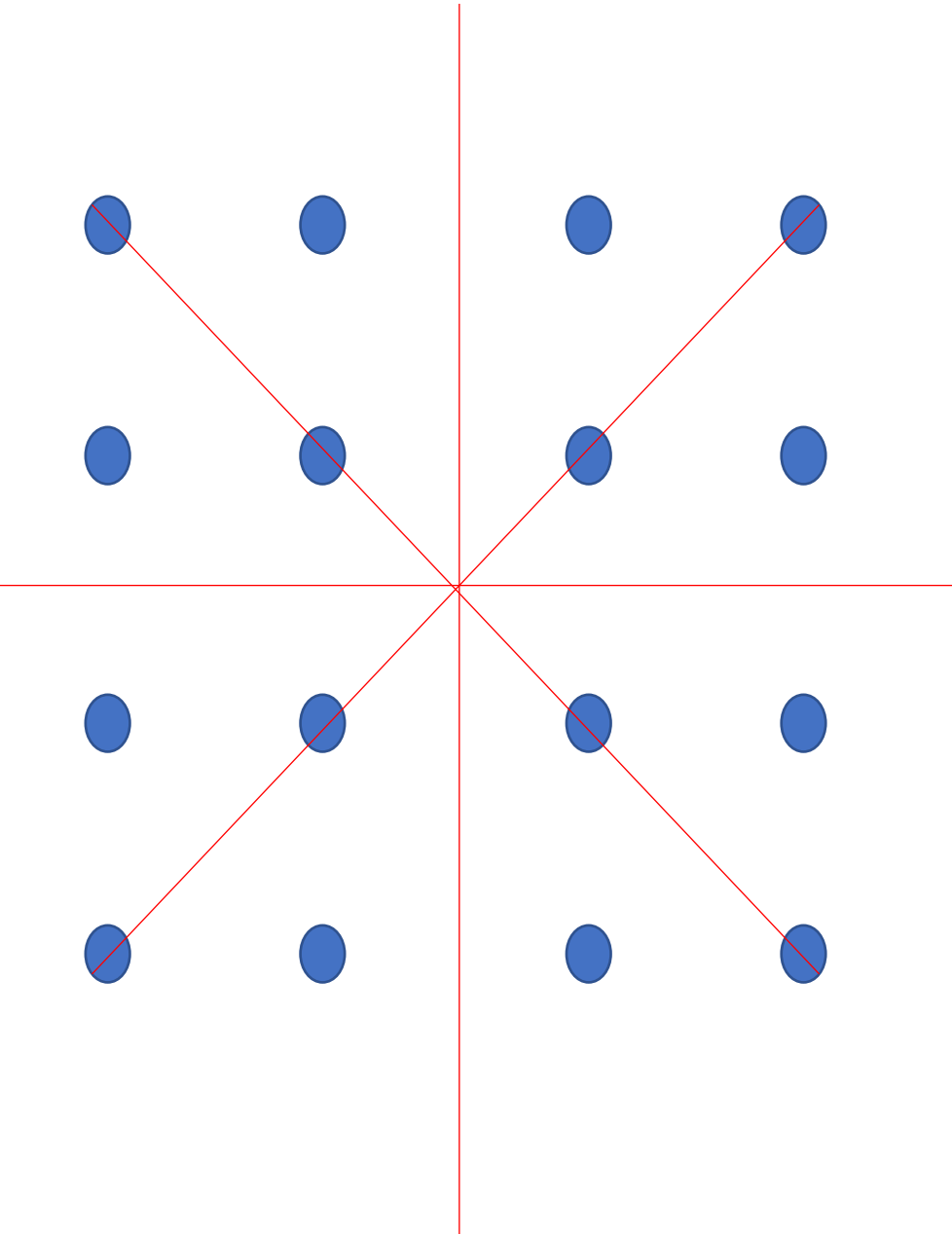
4 crystal systems
5 types of lattices!

Oblique

- Center of inversion (Infact all periodic lattices should atleast have center of inversion)
- $A \neq B$
- No angle restrictions

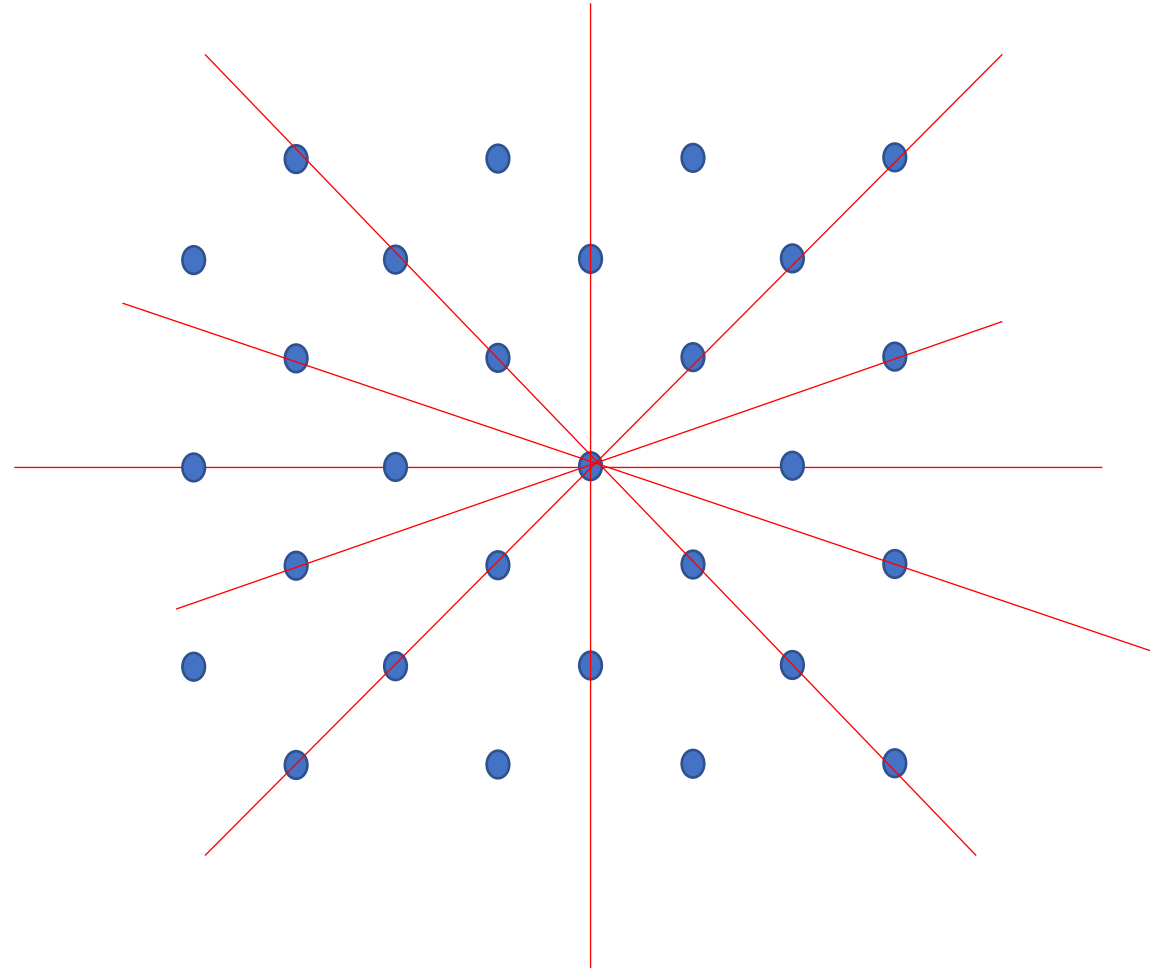


2D Square lattice



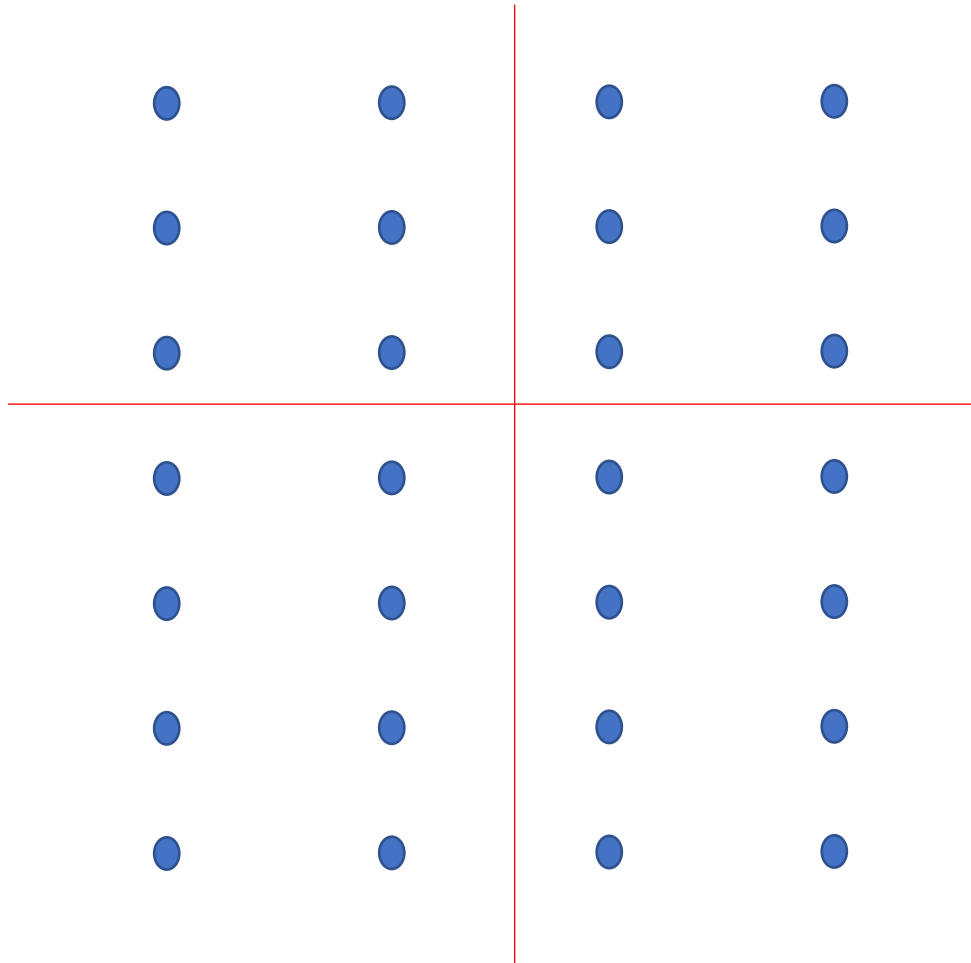
- 4 fold symmetry
 - Rotation by 90
- 4 mirror planes
 - Diagonals and bisectors
- $A = B$
- $\alpha = 90$

Hexagonal 2D



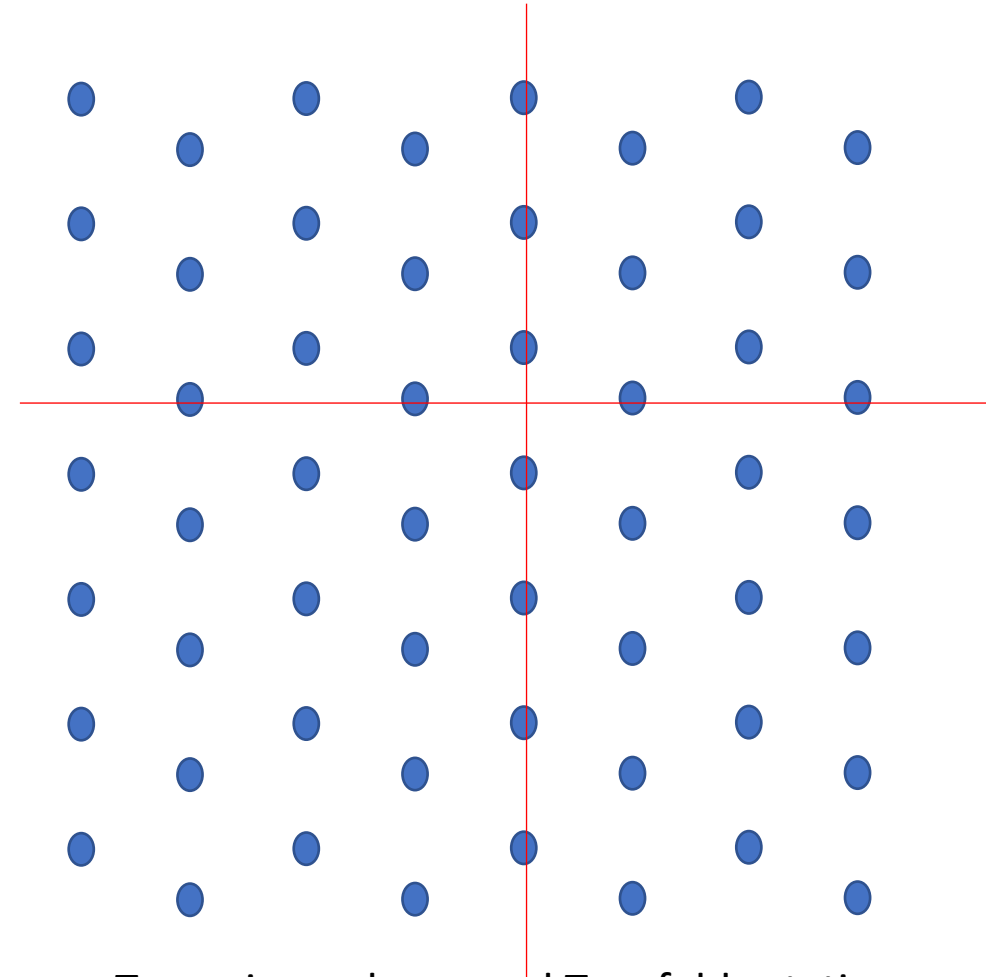
- 6 fold symmetry
- 6 Mirror planes
- $A = B$
- $\alpha = 120$

Rectangle



Two mirror planes and Two fold rotation

Centered Rectangle

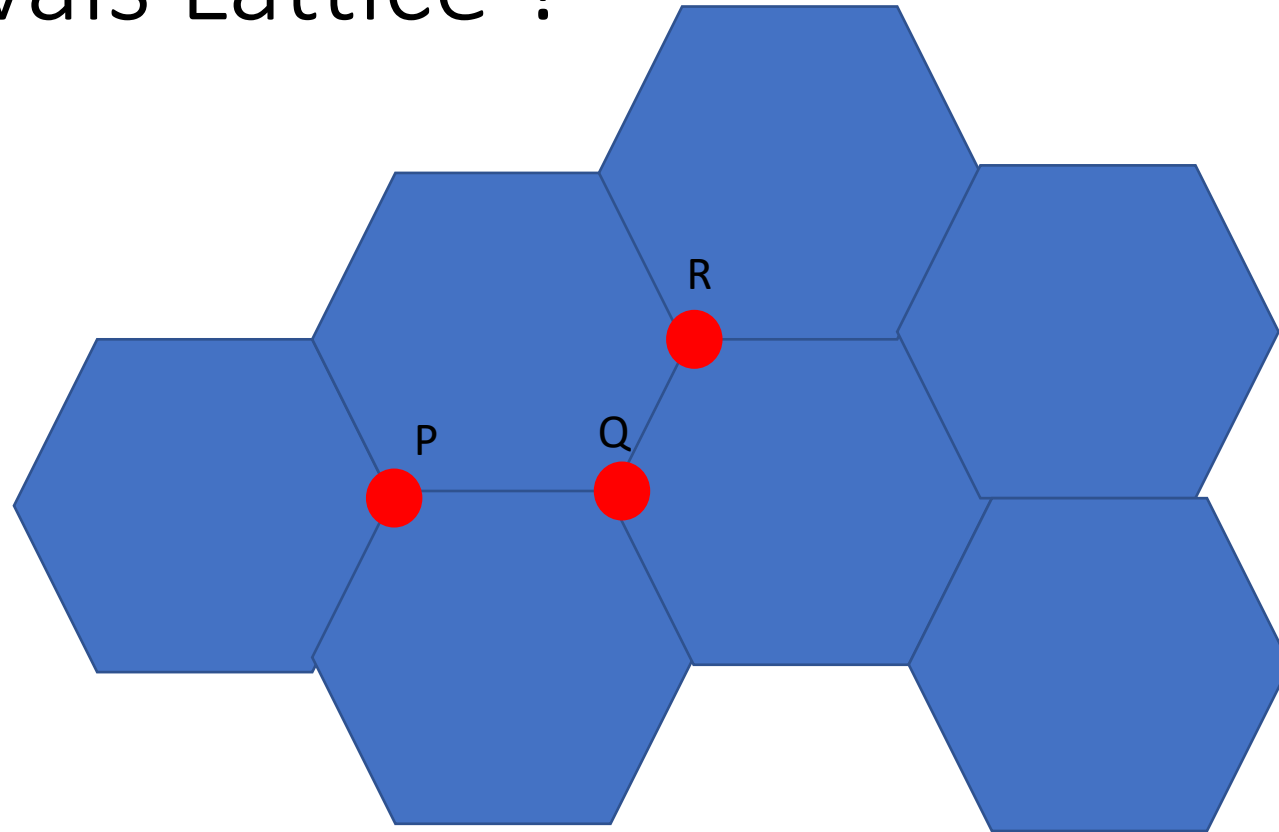


Two mirror planes and Two fold rotation

Unit cells of 2D (Bravais lattices)

Name	Lattice vectors	Symmetry
Oblique	$A \neq B, \alpha \neq 90$	Two-fold rotation/ center of inversion
Square	$A=B, \alpha = 90$	Four fold symmetry, Four mirror planes
Hexagonal	$A=B, \alpha = 120$	Six fold symmetry, 6 mirror planes
Rectangular	$A \neq B, \alpha = 90$	Two fold symmetry, two mirror planes
Centered rectangle	$A \neq B, \alpha = 90$	Two fold symmetry, two mirror planes

Is this a Bravais Lattice ?



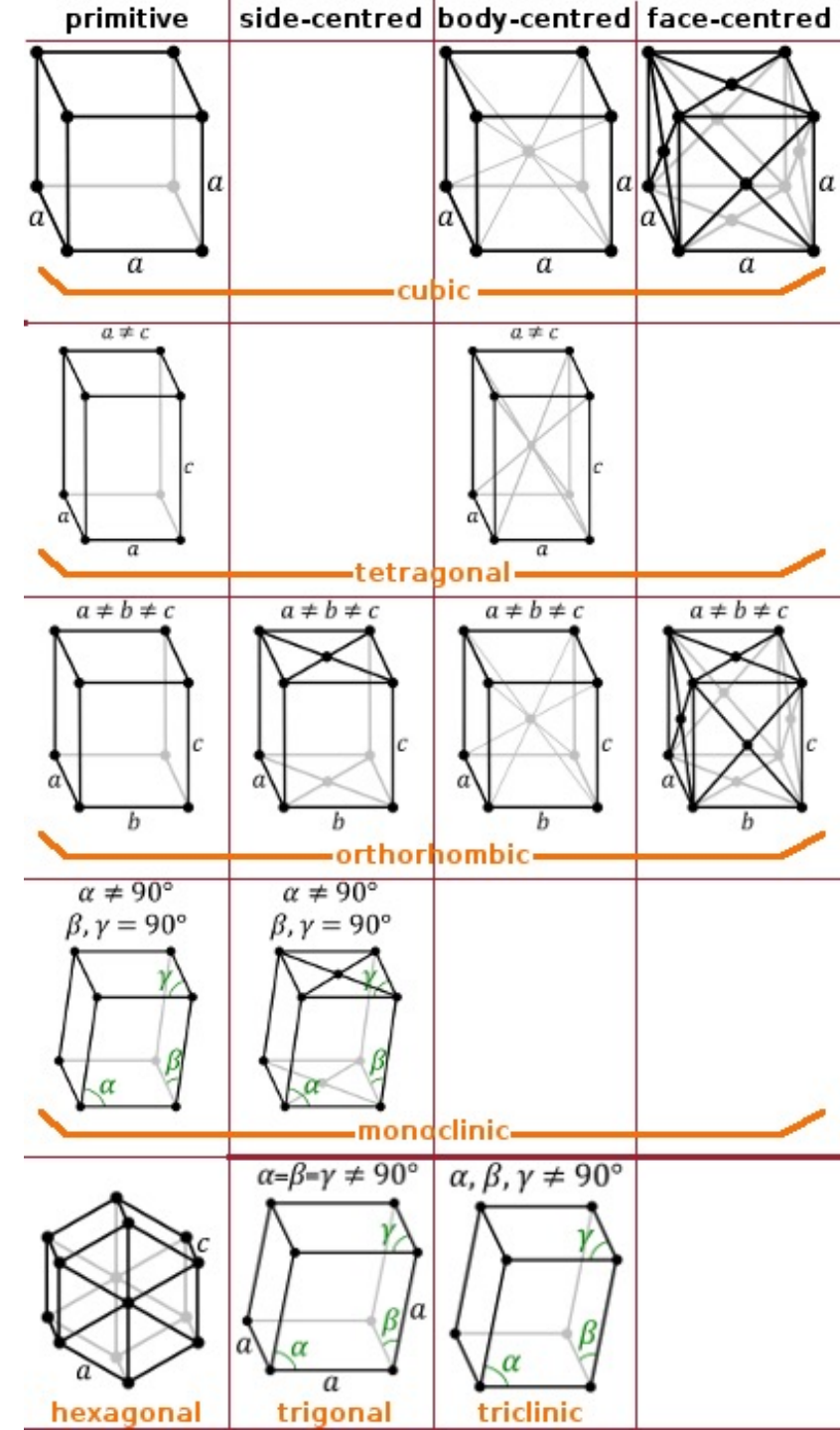
All Points should have the same view !

7 – Bravais lattice types

- 14 lattices

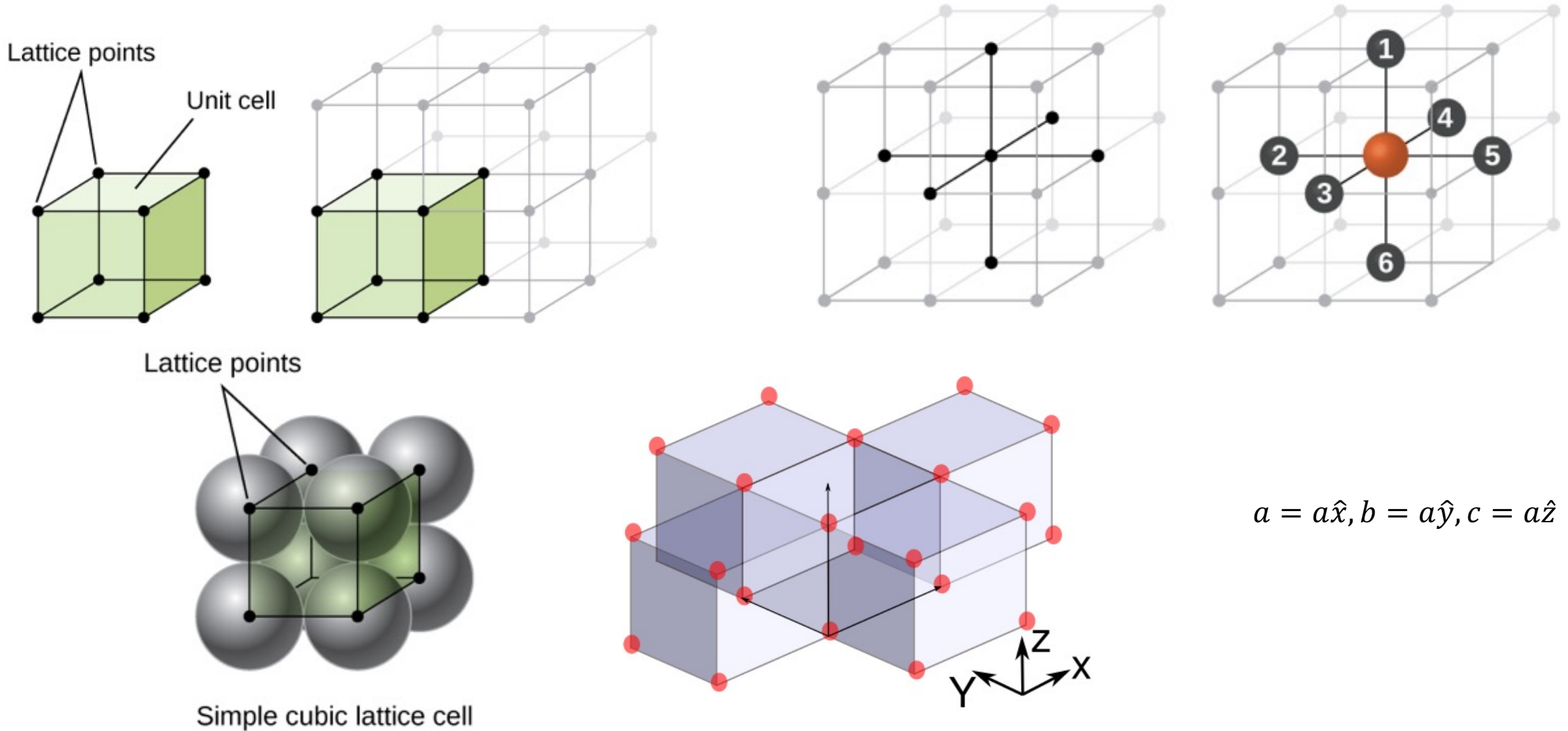
Coordinate systems of crystals = **7 crystal systems in 3 dim.**

Name of system	Minimum symmetry	Conventional unit cell
triclinic	1 or -1	$a \neq b \neq c; \alpha \neq \beta \neq \gamma$
monoclinic	<u>one</u> diad – 2 or m ($\parallel Y$)	$a \neq b \neq c; \alpha = \gamma = 90^\circ, \beta > 90^\circ$
orthorhombic	<u>three</u> mutually perpendicular diads – 2 or m ($\parallel X, Y$ and Z)	$a \neq b \neq c; \alpha = \beta = \gamma = 90^\circ$
tetragonal	<u>one</u> tetrad – 4 ($\parallel Z$)	$a = b \neq c; \alpha = \beta = \gamma = 90^\circ$
trigonal (hexagonal cell)	<u>one</u> triad – 3 or -3 ($\parallel Z$)	$a = b \neq c; \alpha = \beta = 90^\circ, \gamma = 120^\circ$
hexagonal	<u>one</u> hexad – 6 or -6 ($\parallel Z$)	$a = b \neq c; \alpha = \beta = 90^\circ, \gamma = 120^\circ$
cubic	<u>four</u> triads – 3 or -3 ($\parallel$ space diagonals of cube)	$a = b = c; \alpha = \beta = \gamma = 90^\circ$



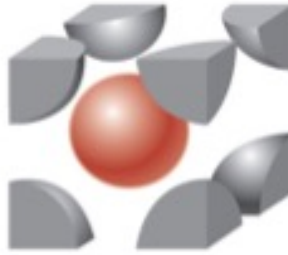
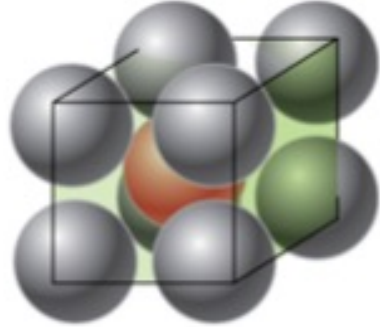
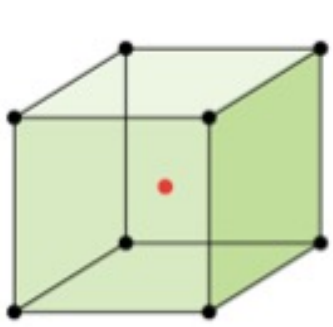
Cubic Systems

3D crystal structures – Simple Cube

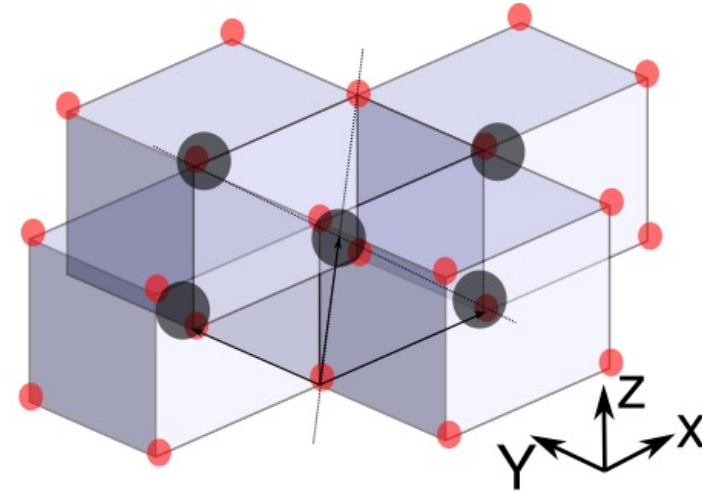
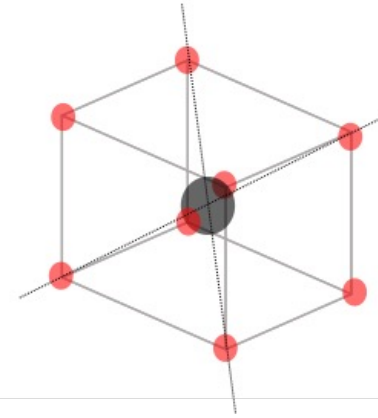


Simple cubic

- An atom at each edge of the cube
- 8 Atoms shared by 8 adjacent cubes
- Empty spaces between the atoms
- 1 atom per unit cell
- Po crystalizes in this form
- Packing fraction = 0.52
- Coordination number is 6



Body-centered cubic structure

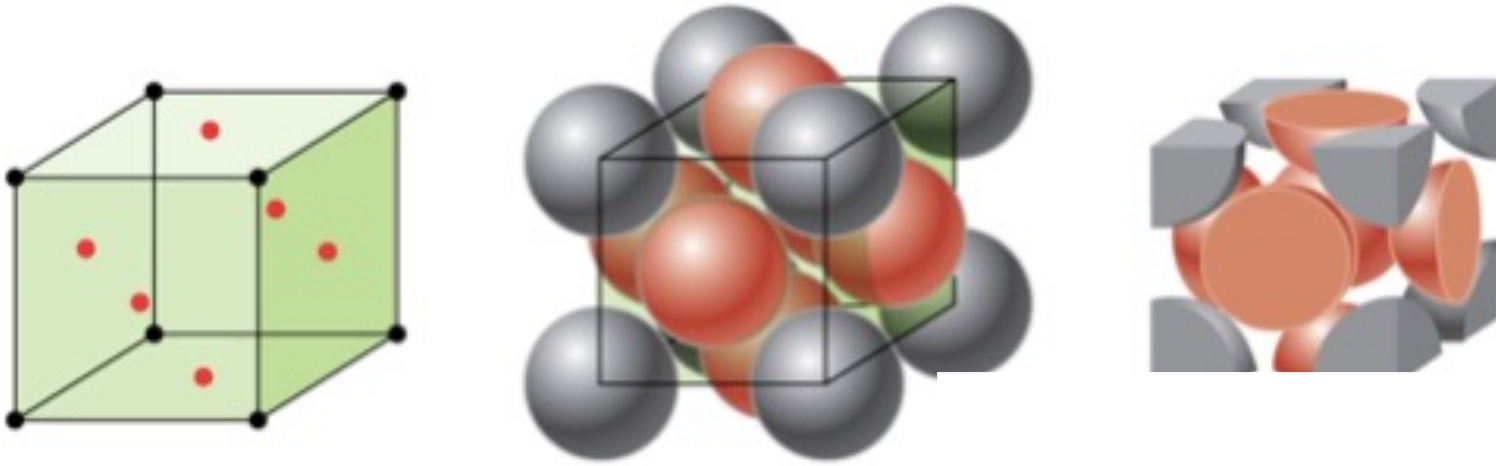


- Total number of atoms per unit cell = $8 \cdot \frac{1}{8} + 1$
- Atoms occupy 68% of the cell volume
- Coordination number is 8
- K, Ba, Cr, Wo, W and Fe crystallize under BCC

Primitive vectors

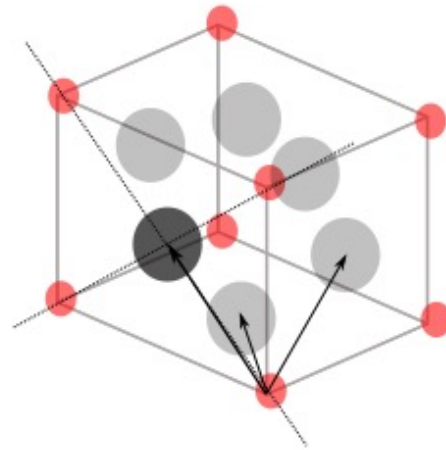
$$a = a\hat{x}, b = a\hat{y}, c = \frac{a}{2}(\hat{x} + \hat{y} + \hat{z})$$

$$a = \frac{a}{2}(\hat{y} + \hat{z} - \hat{x}), b = \frac{a}{2}(\hat{x} + \hat{z} - \hat{y}), c = \frac{a}{2}(\hat{y} + \hat{x} - \hat{z}),$$



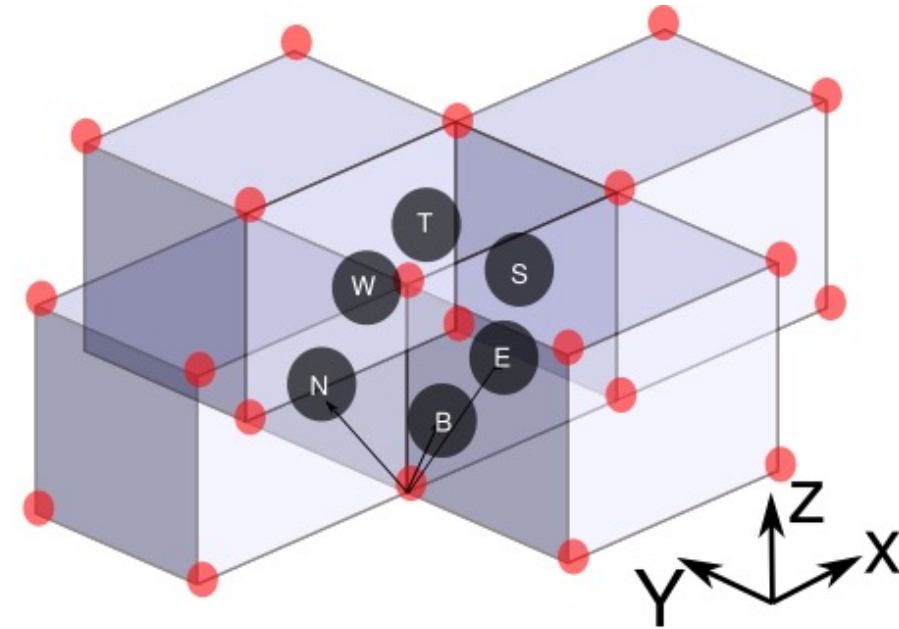
Face-centered cubic structure

- Corner atoms contribute $\frac{1}{8} \times 8$
- Face atoms contribute $6 \times \frac{1}{2}$
- Also called as Cubic closed pack
- Coordination number 12
- Atoms occupy about 74% of the unit cell volume



Primitive vectors

$$a = \frac{a}{2}(\hat{y} + \hat{z}), b = \frac{a}{2}(\hat{x} + \hat{z}), c = \frac{a}{2}(\hat{y} + \hat{x})$$



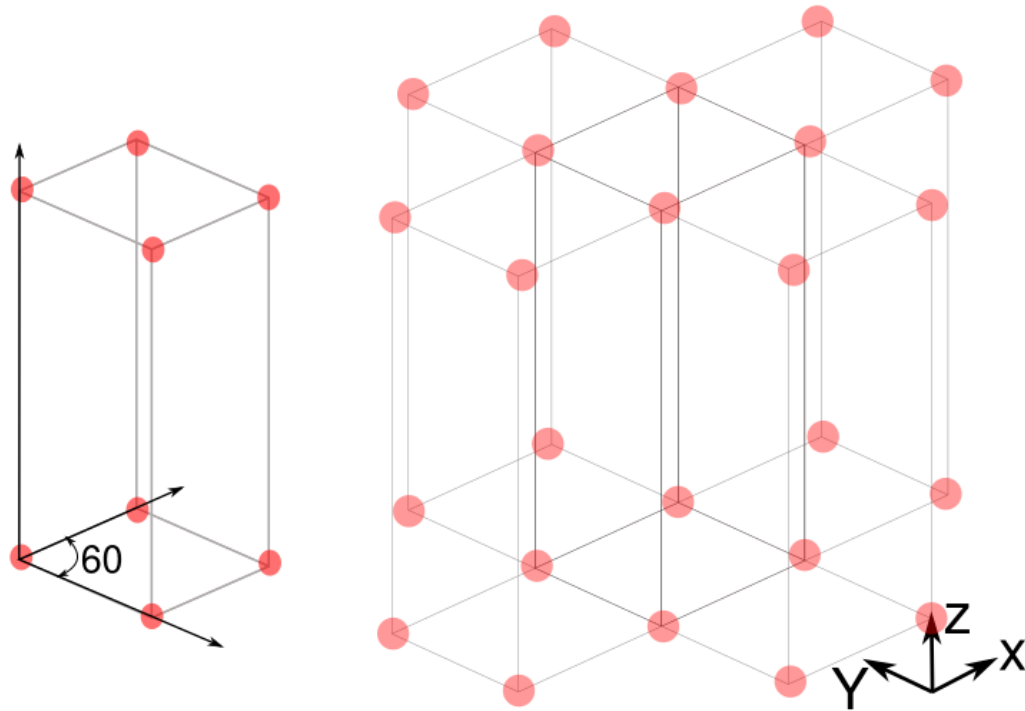
Examples: Au, Ag, Cu, Al, Ca ...

characteristics of cubic crystal

	Parameters	Simple Cubic	Body centered	Face centered
1	Lattice constant (a)	$a = 2r$	$a = \frac{4}{\sqrt{3}}r$	$a = \frac{4}{\sqrt{2}}r$
2	Volume of unit cell (V)	a^3	a^3	a^3
3	Number of lattice point (atom) per unit cell	1	2	4
4	Volume of primitive cell	a^3	$a^3/2$	$a^3/4$
5	Coordinate number (Number of nearest neighbors)	6	8	12
6	nearest neighbors distance	a	$\frac{\sqrt{3}}{2}a$	$\frac{1}{\sqrt{2}}a$
7	Packing fraction (PF)	$\frac{\pi}{6} = 0.52$	$\frac{\sqrt{3}\pi}{8} = 0.68$	$\frac{\pi}{3\sqrt{2}} = 0.74$

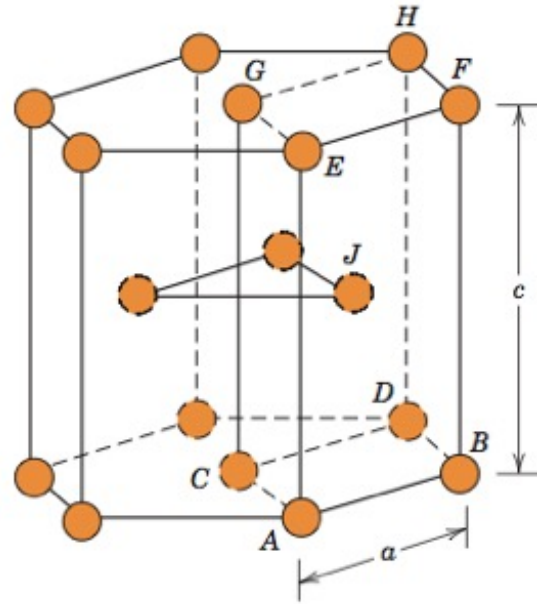
Hexagonal Systems

Hexagonal

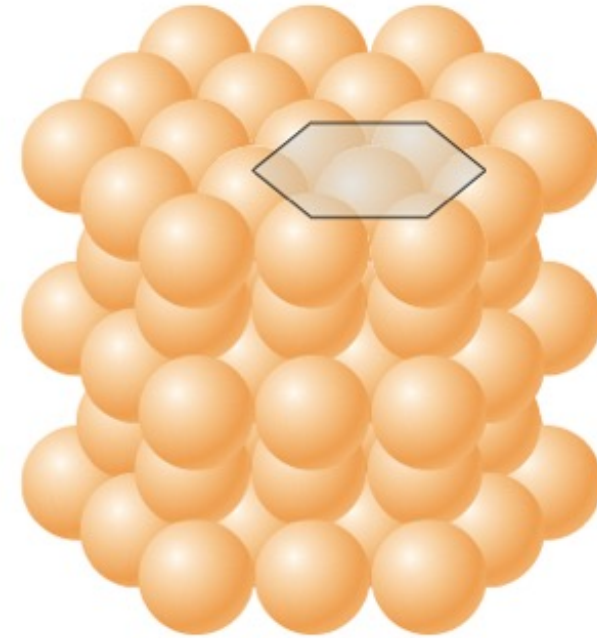


$$a = a\hat{x}, b = \frac{a}{2}\hat{x} + \frac{\sqrt{3}a}{2}\hat{y}, c = c\hat{z}$$

Hexagonal Closed Pack



$$\vec{a}_1 = \frac{a}{2}\hat{x} + \frac{\sqrt{3}a}{2}\hat{y}, \quad \vec{a}_2 = \frac{a}{2}\hat{x} - \frac{\sqrt{3}a}{2}\hat{y}, \quad \vec{a}_3 = c\hat{z}$$



Co, Cd, Zn, Ti

Wigner-Seitz cell

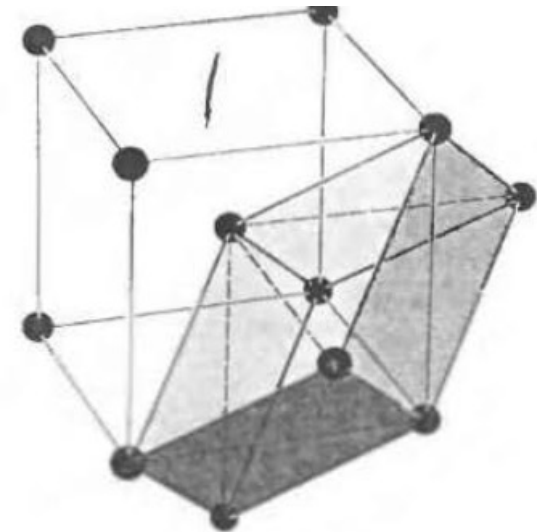
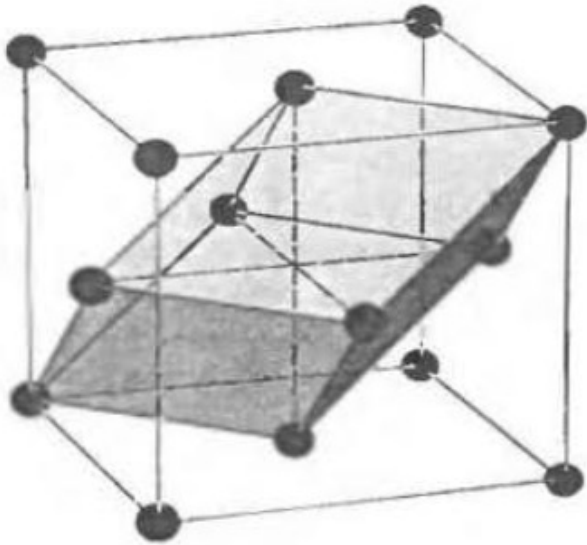
A primitive cell must contain only one lattice point per unit cell

If there are N points per cm^3 , ie N is the density of lattice points,

Then, $N * v = 1$ or $v = 1/N$

Since, this holds for any primitive cell, The volume of a primitive cell must be constant

However, the primitive cell can have lower symmetry than the unit cell. One example is the FCC shown below

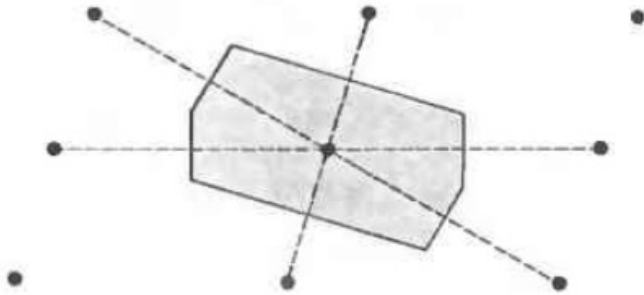


Solid State Physics, Ashcroft and Mermin

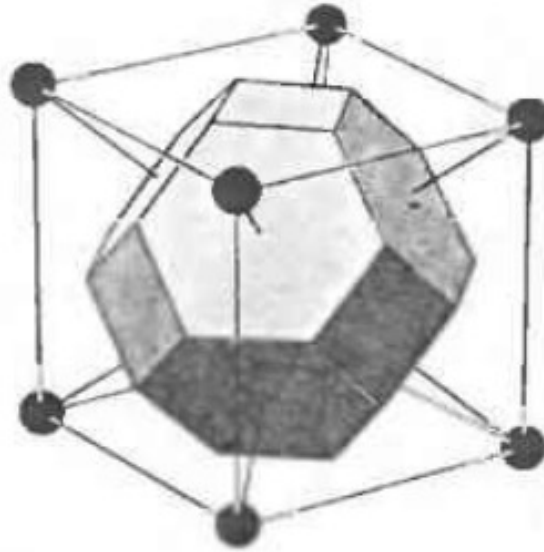
Wigner-Seitz cell

A primitive cell with full symmetry of the Bravais Lattice is called as Wigner-Seitz cell.

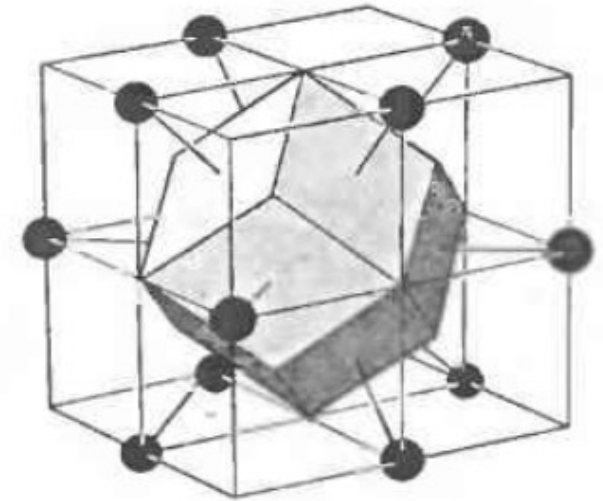
Since the previous definitions of primitive cells depends on the choice of the basis vectors, it can have lower symmetry. However, WS is formed by only nearest neighbors.



Case of simplest Wigner-Seitz Cell



BCC - WS

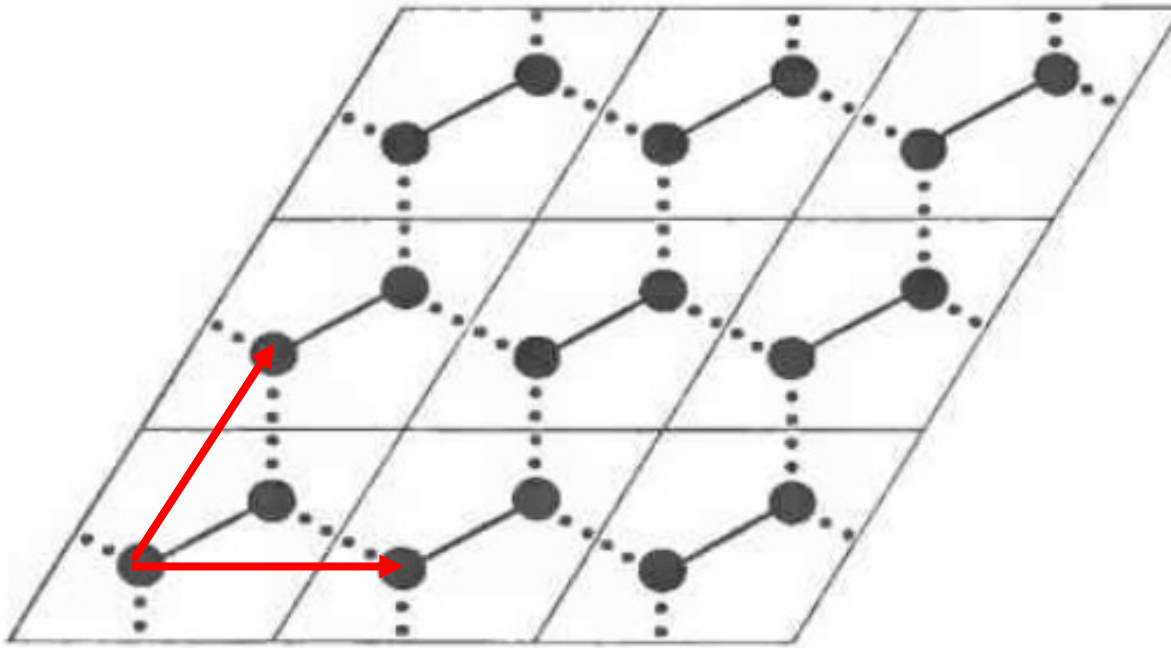


FCC - WS

Primitive cell - one atom per volume. Same symmetry as the unit cell

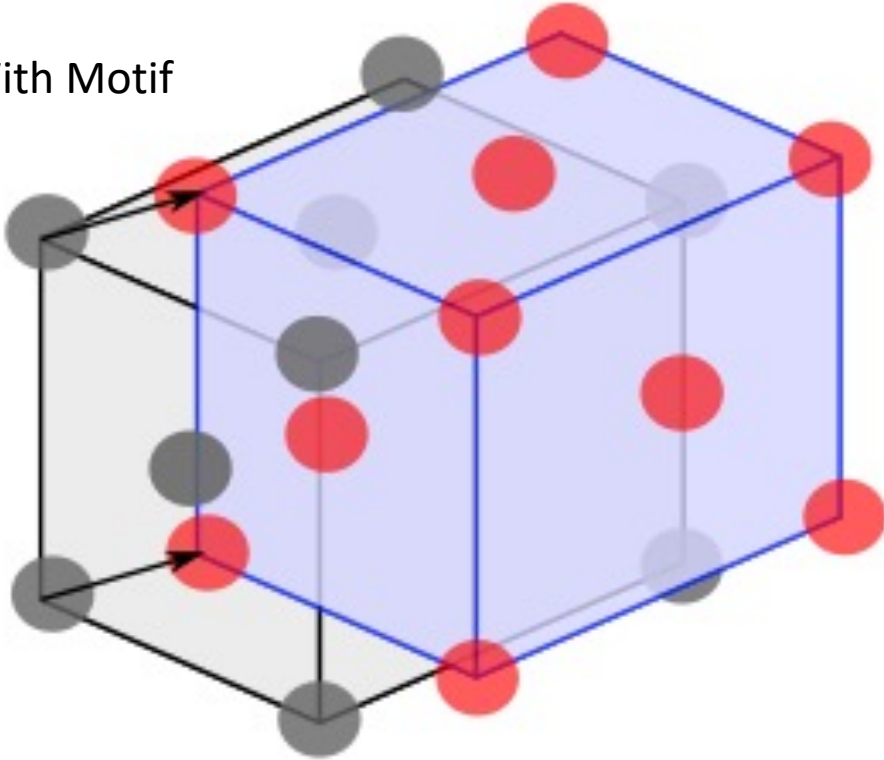
Crystal Structure

- Lattice is a mathematical collection of points
- Lattice + atomic cluster gives crystal structure

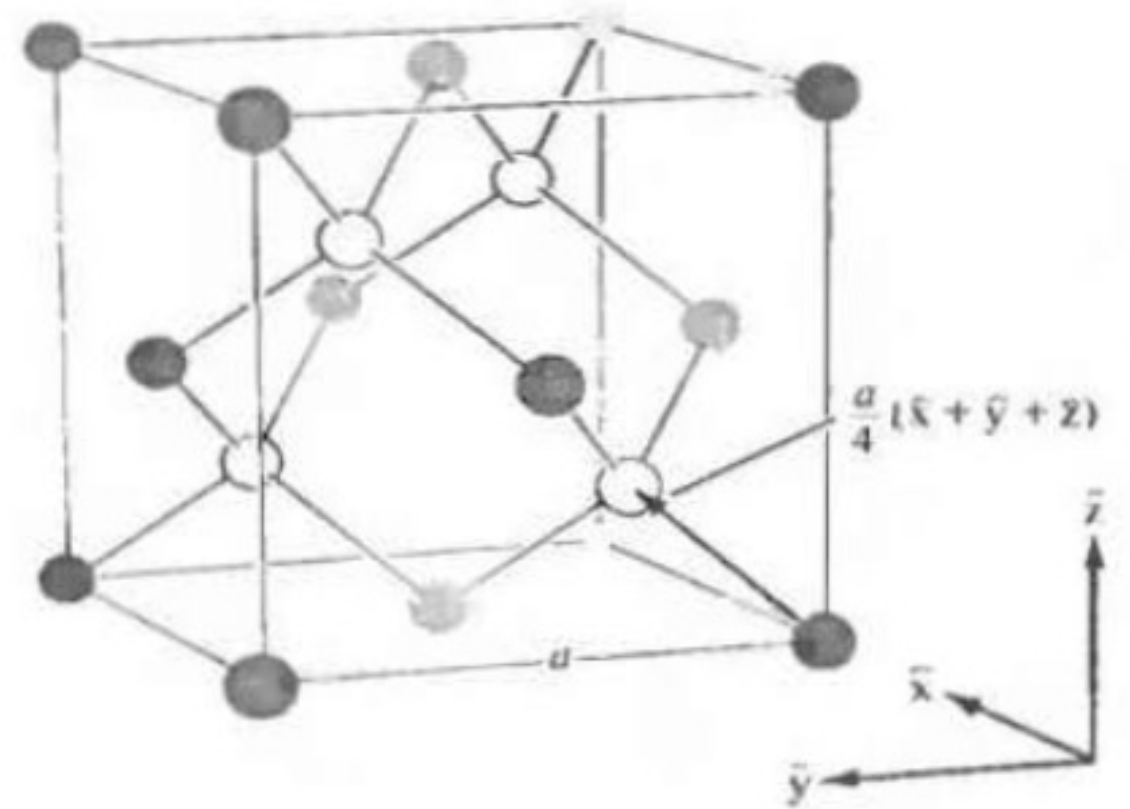


Diamond Lattice

FCC With Motif



Atoms at 0 and $\frac{a}{4}(\vec{x} + \vec{y} + \vec{z})$

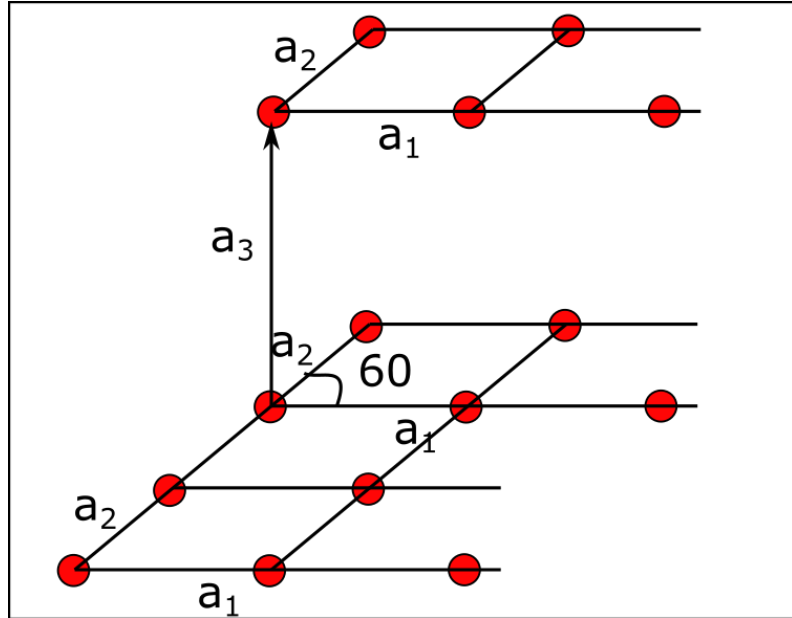


Elements with Diamond structure:

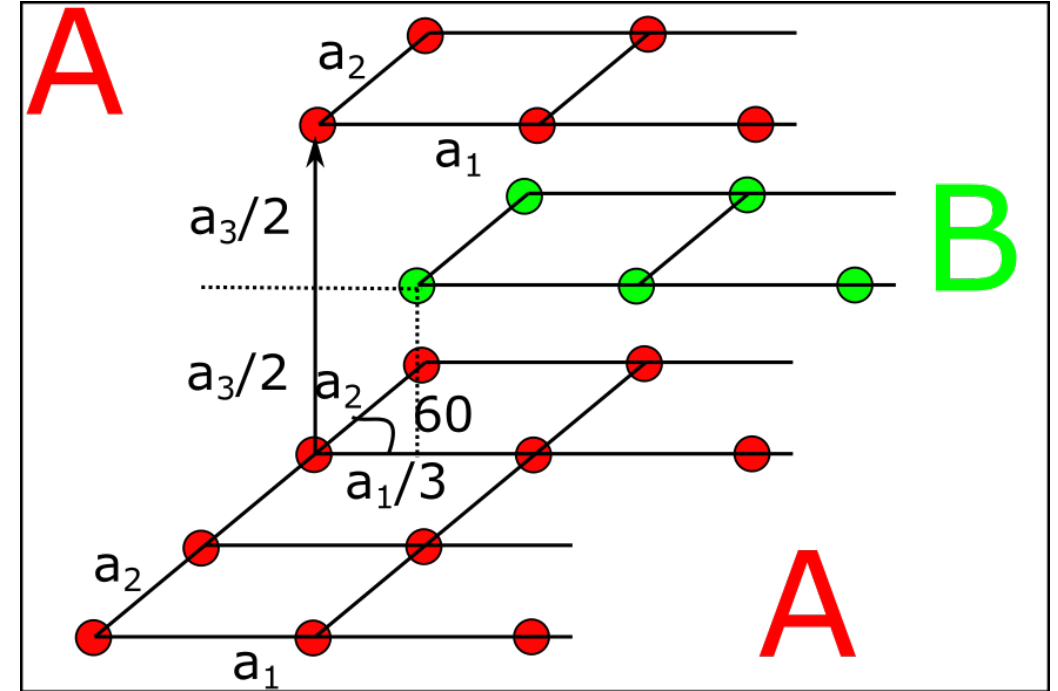
1. Diamond (3.57 Å)
2. Si (5.43 Å)
3. Ge (5.66 Å)

Solid State Physics, Ashcroft and Mermin

Hexagonal Closed Pack



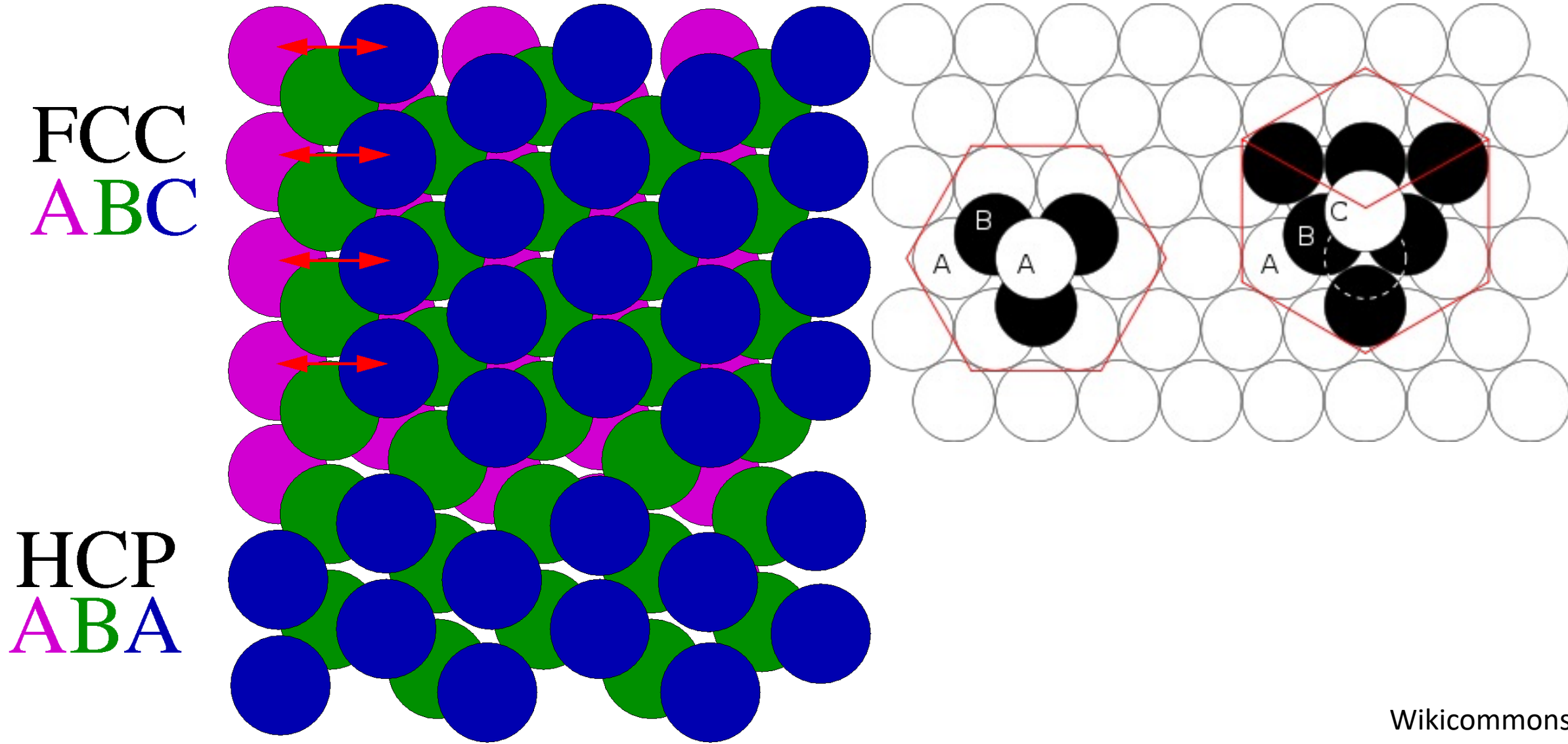
Element	A	B	c/a
Be	2.29	3.58	1.56
Hf	3.20	5.06	1.58
Y	3.65	5.73	1.57
Ideal			$c = \sqrt{\frac{8}{3}} a$ $= 1.63 a$



Hexagon with a motif

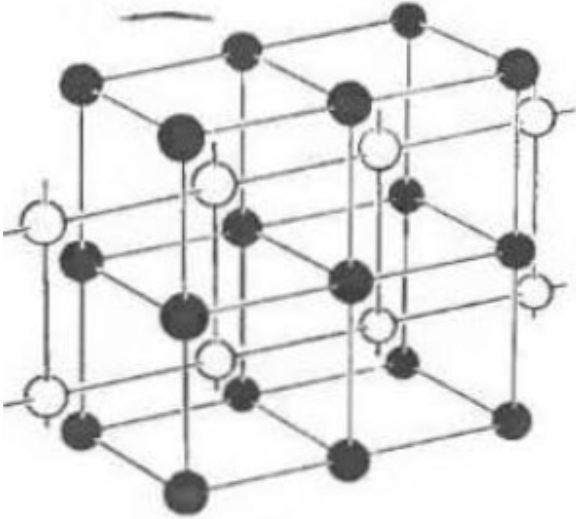
HCP vs FCC

Comparison of closed pack structures



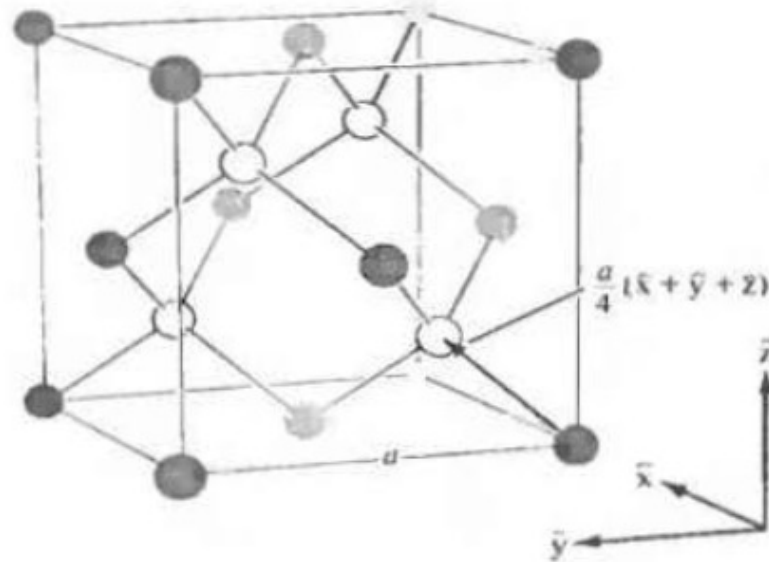
Lattice with a Motif

Simple Cube + Motif



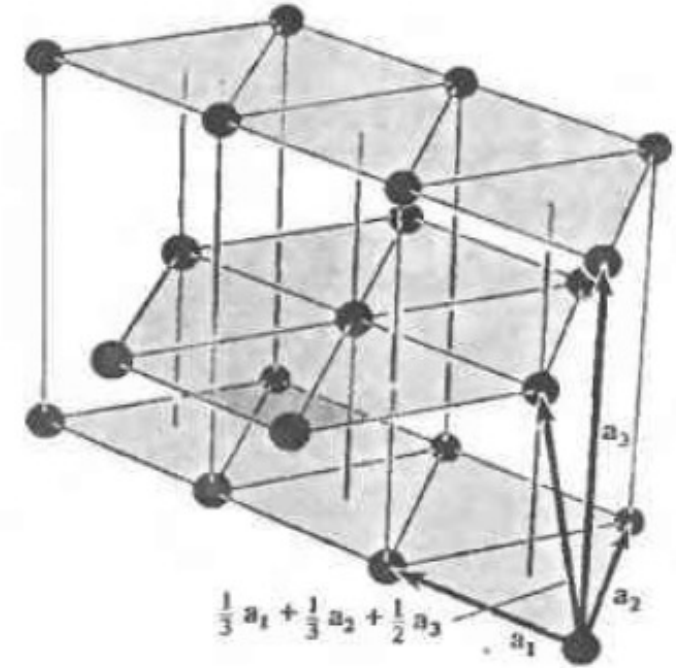
Example: CsCl

FCC with motif



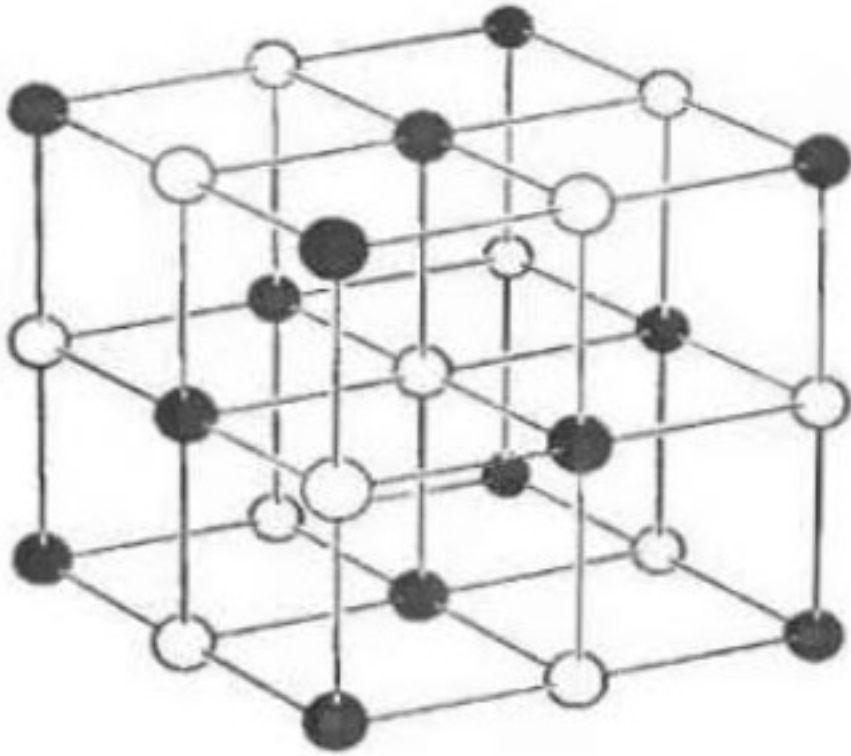
Same atoms: Si, Ge, Diamond
Different atoms: ZnS, GaAs, InP,

Hexagonal with motif



Example: Quartz

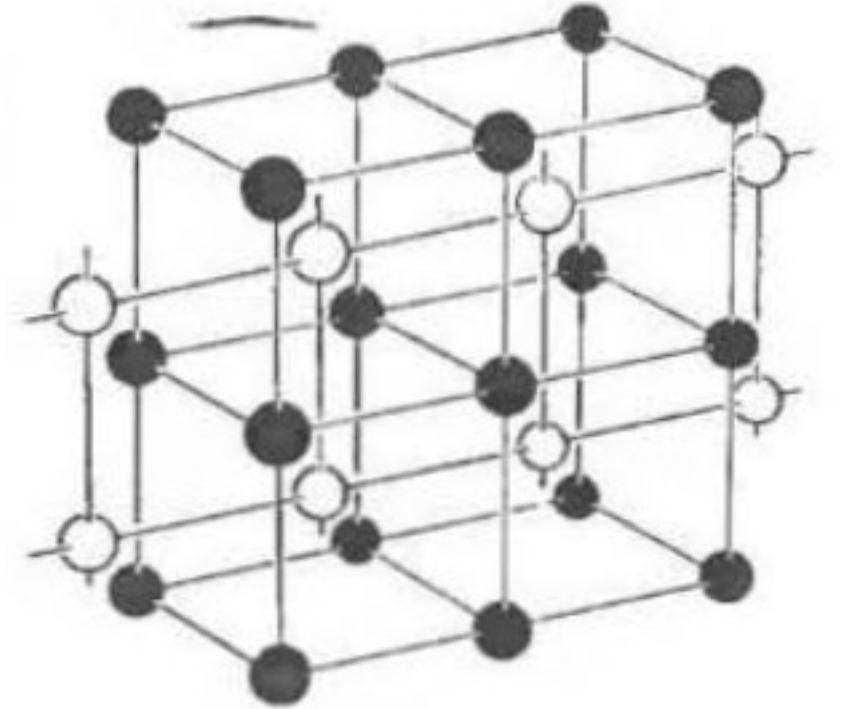
NaCl Structure and CsCl



Face centered cube Bravais lattice with motif at body center

Lattice with motif at $0, \frac{A}{2}(\vec{x} + \vec{y} + \vec{z})$

Eg: NaCl, KCl, LiF, NaF, Many such ionic salts

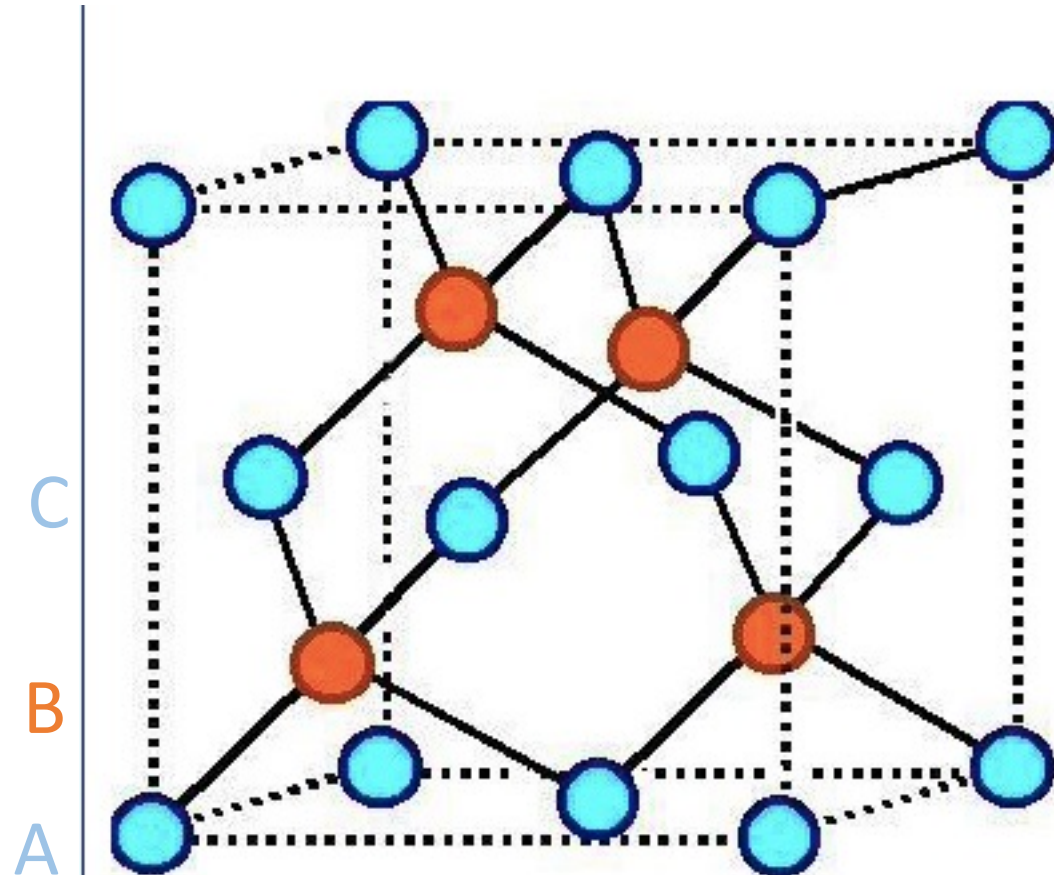


Simple cube Bravais lattice with motif at body center

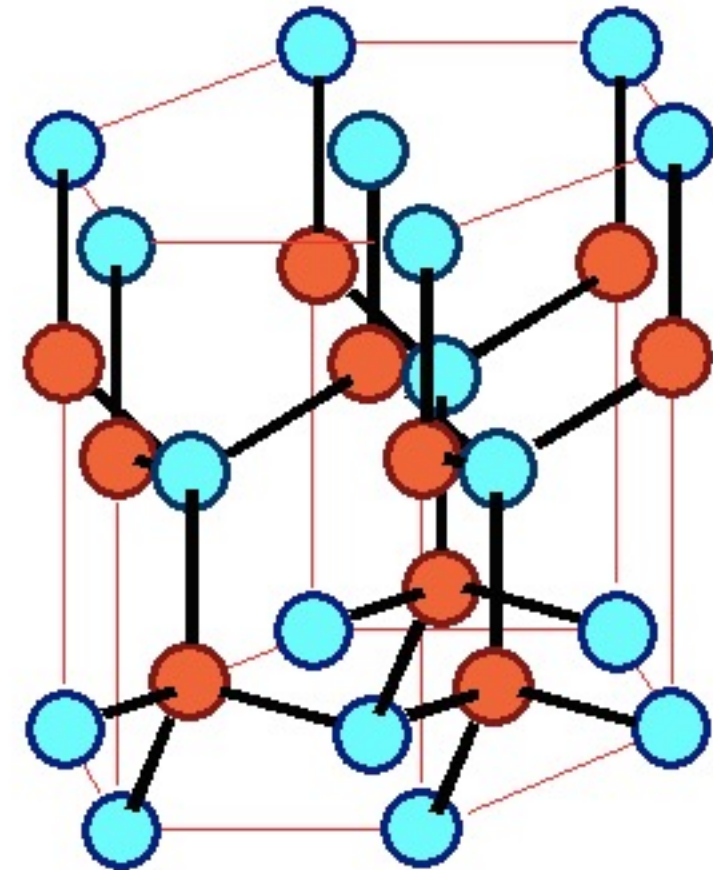
$0, \frac{A}{2}(\vec{x} + \vec{y} + \vec{z})$

CsCl, CsBr, CsI and such

Zinc Blende and Wurtzite

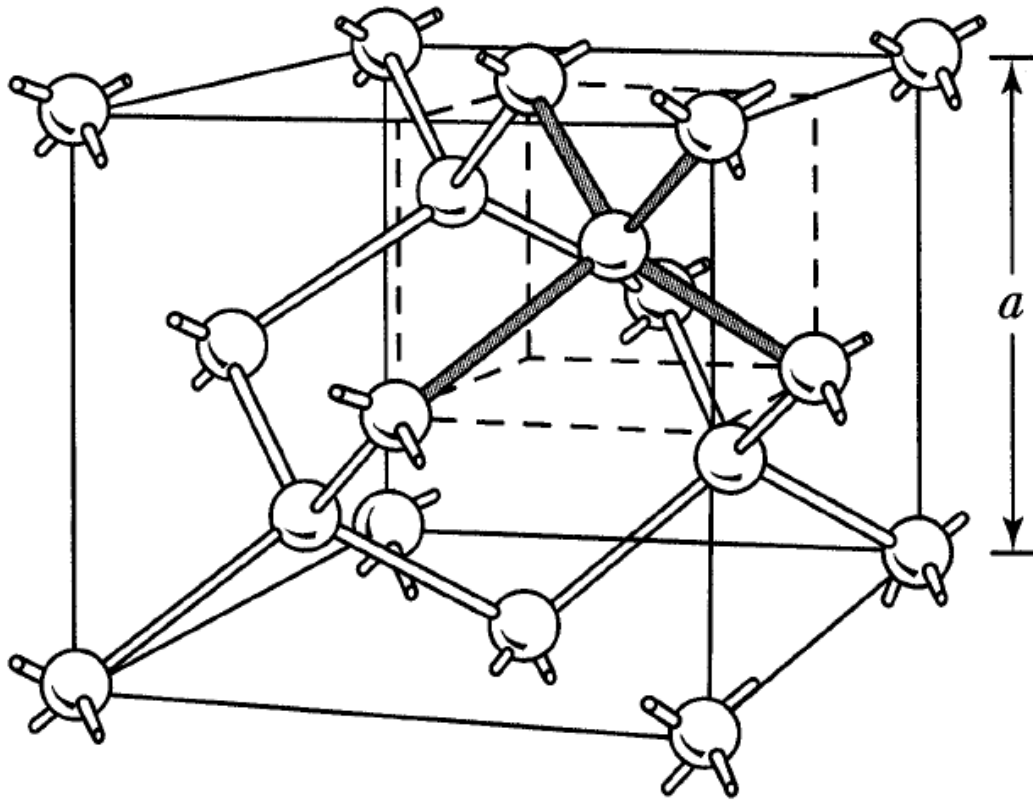


**Zinc blende or sphalerite
or Diamond structure**

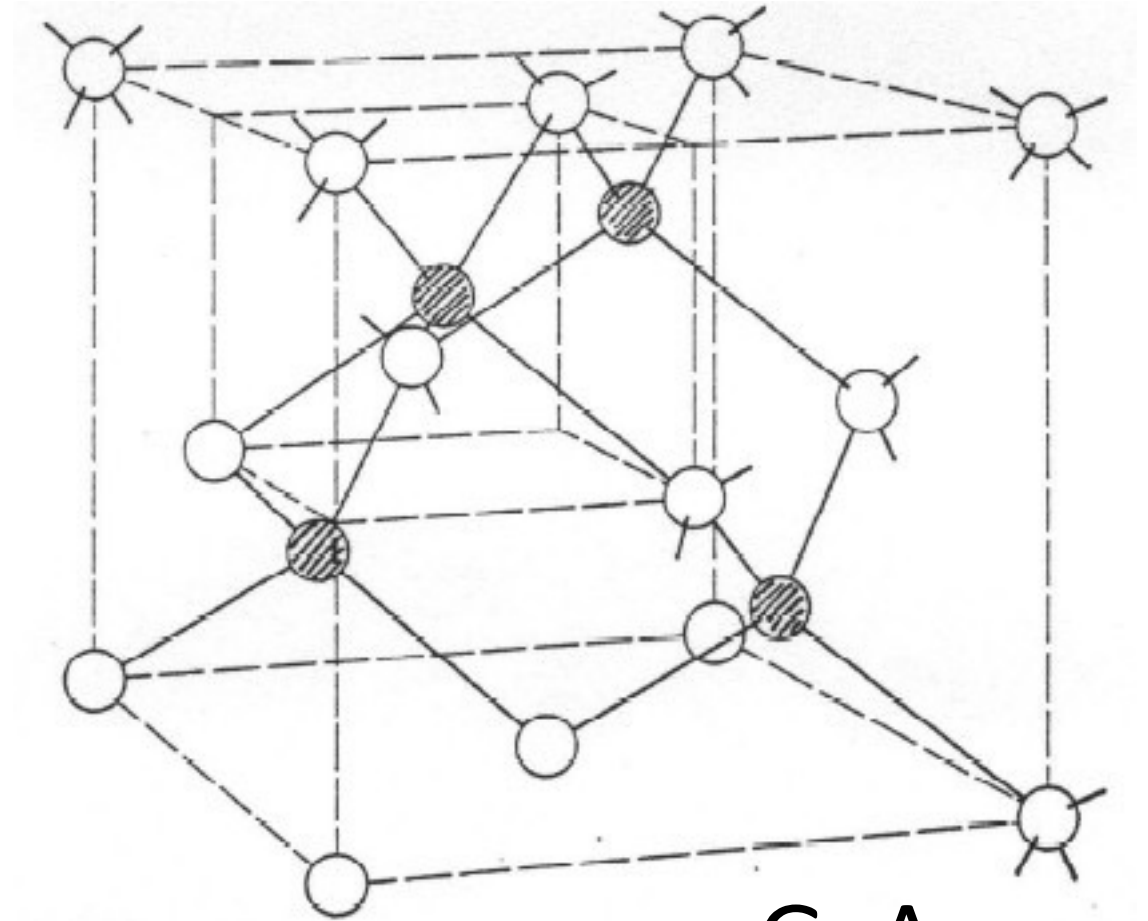


**Wurtzite
or hexagonal structure**
Red lines are not showing bonds.

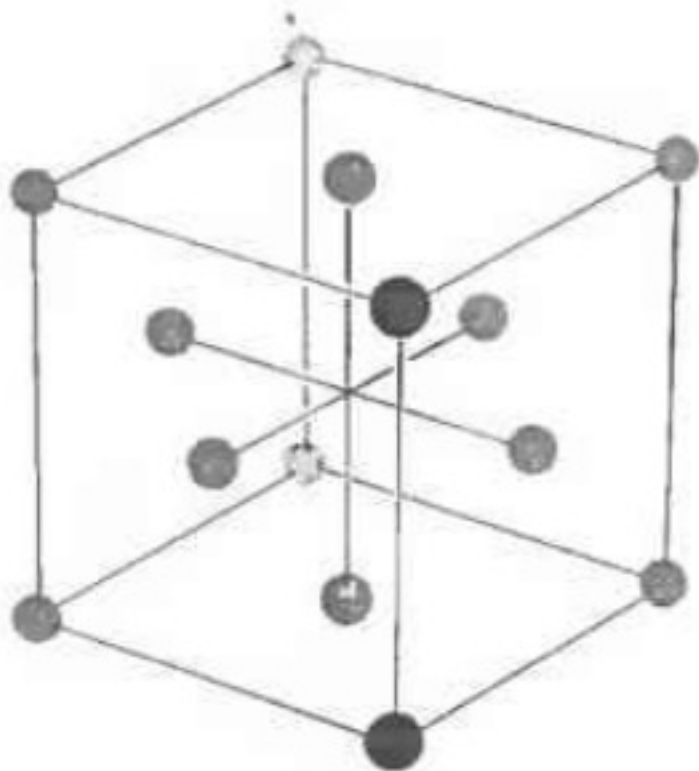
Crystal Structures of common Materials



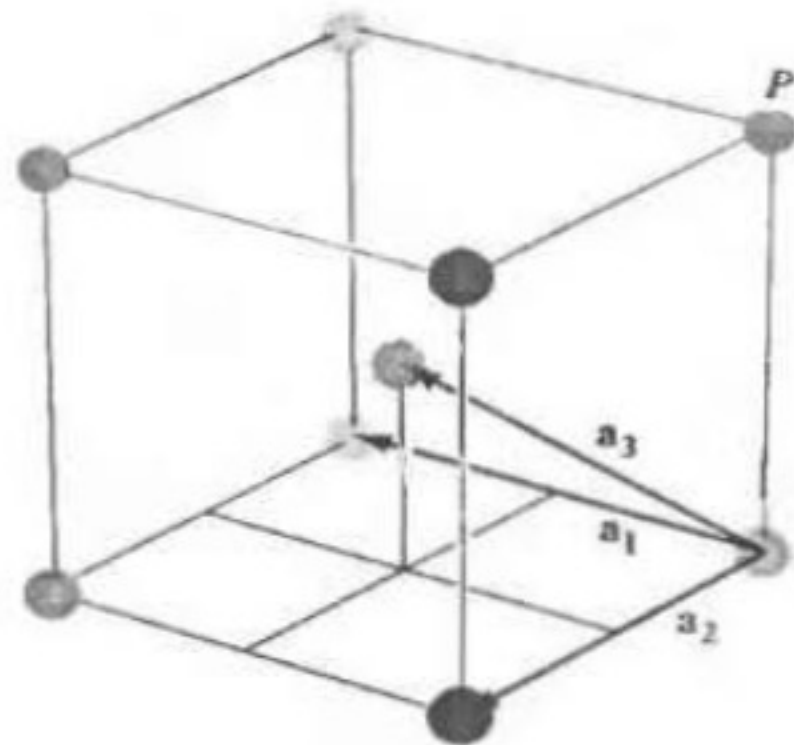
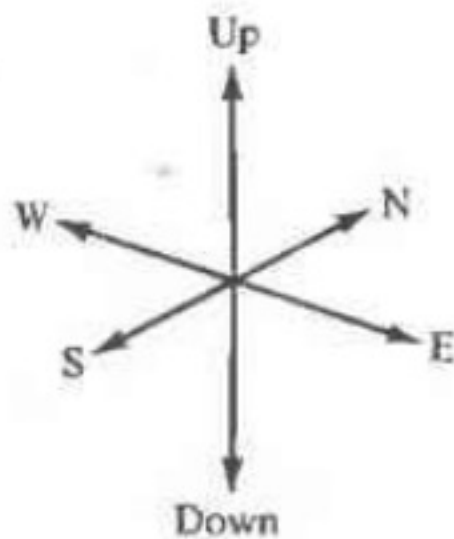
Si



GaAs



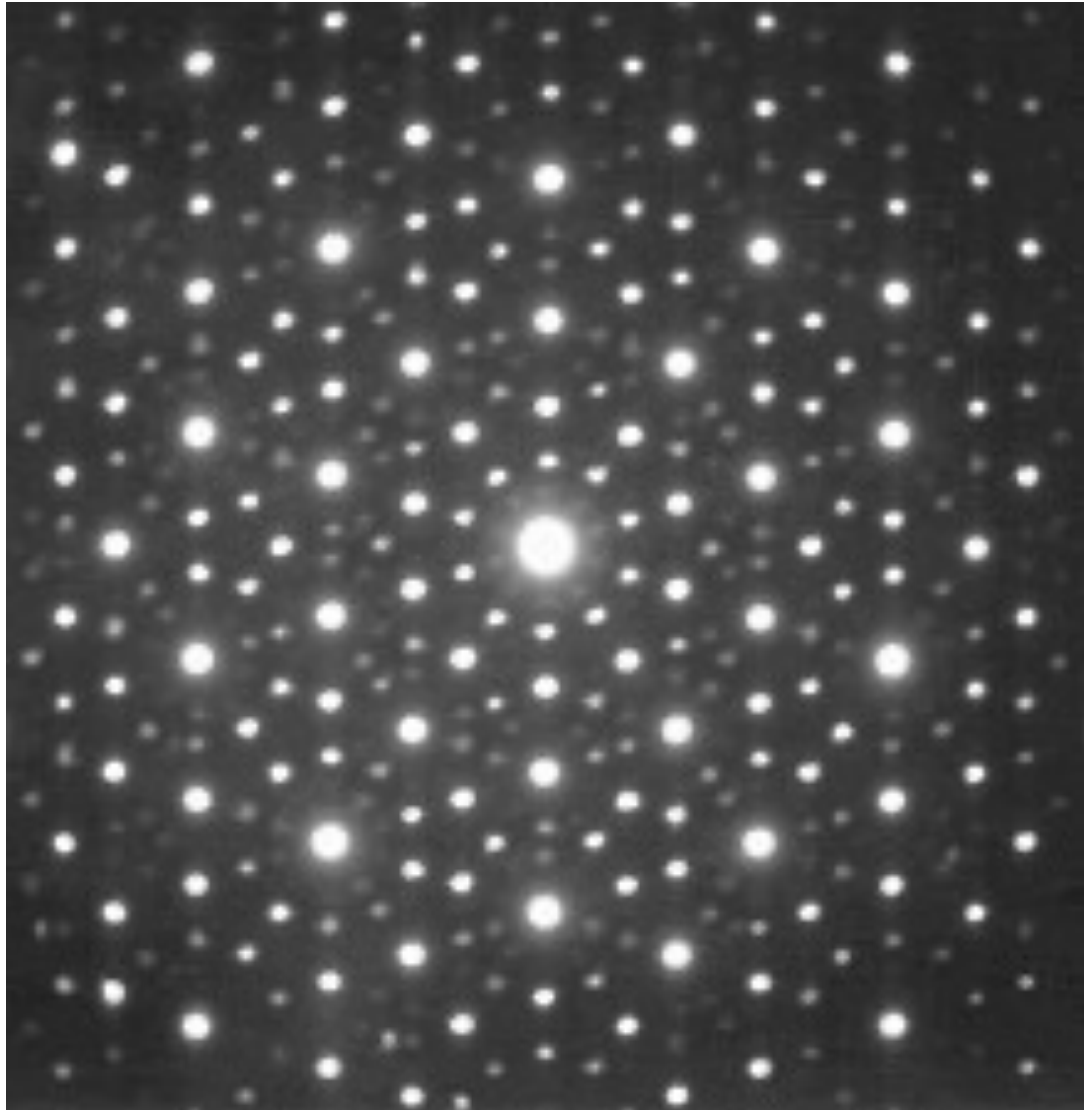
Au, Cu, Ag...



Fe, K, Be,...

$$a_1 = a\lambda_1$$

So what about quasi s ?



Penrose Tiles

