Crystal Structure

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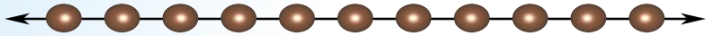
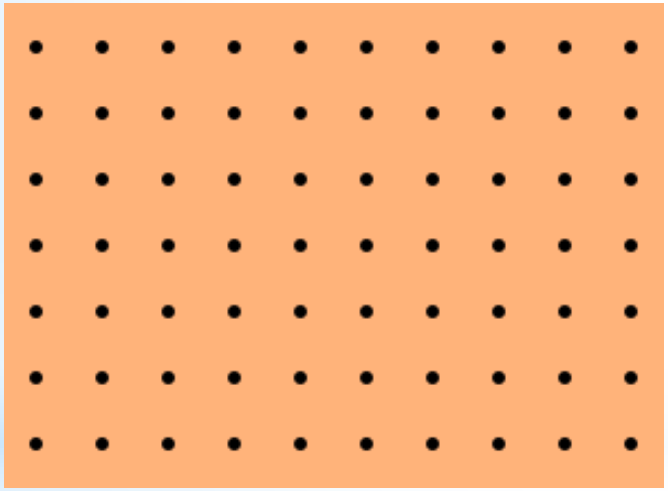
Lattice: In 1848 Bravais introduced the concept of space lattice. Lattice is an imaginary mathematical concept.

“Lattice is an infinite, periodic array of points in space arranged such that the points about any given point are arranged identically with that about any other point.”

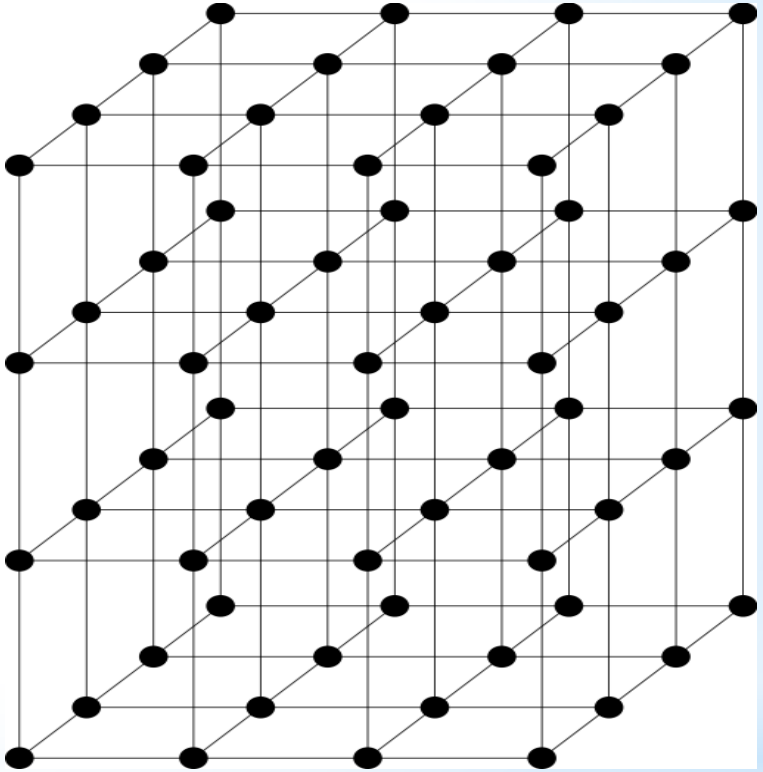
It may consider as removal of the atom but the center remains there.



1D or Linear lattice



2D or Planer lattice

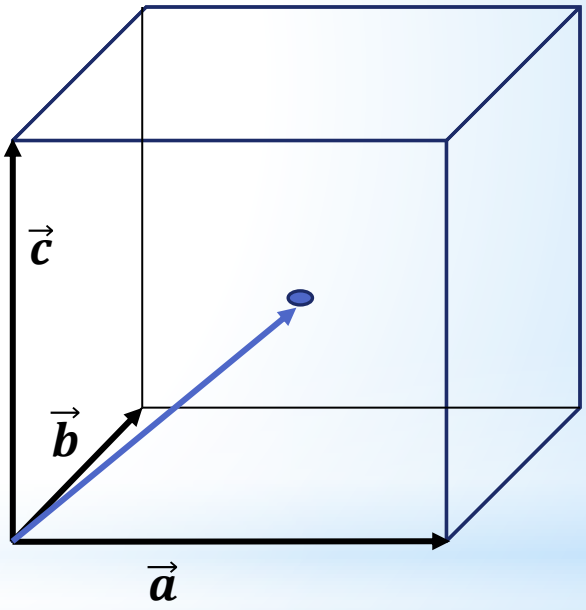


3D or Space lattice

Translation Vector: Lattice is a mathematical abstraction which is defined by 3 fundamental translation vectors $\vec{a}$, $\vec{b}$, $\vec{c}$ along 3 crytallographic directions, X, Y and Z, such that the atomic arrangement looks the same in every respect when viewed from the point $\vec{r}$ as when viewed from the point $\vec{r'}$.

$$\vec{r'} = \vec{r} + n_1\vec{a} + n_2\vec{b} + n_3\vec{c} \quad \ldots\ldots\ldots\ldots\ldots\ldots (1)$$

Where n_1, n_2, n_3 are arbitrary integers and the set of points $\vec{r'}$ defined by (1) for all n_1, n_2, n_3 defines a lattice.



Lattice point can thus be defined by 3-fundmental basis vectors called primitive translation vector in X, Y, Z crystallographic direction as

$$\vec{\tau} = n_1\vec{a} + n_2\vec{b} + n_3\vec{c} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots (2)$$

So that $\vec{r'} = \vec{r} + \vec{\tau}$, Here, $\vec{\tau}$ is the translation vector.

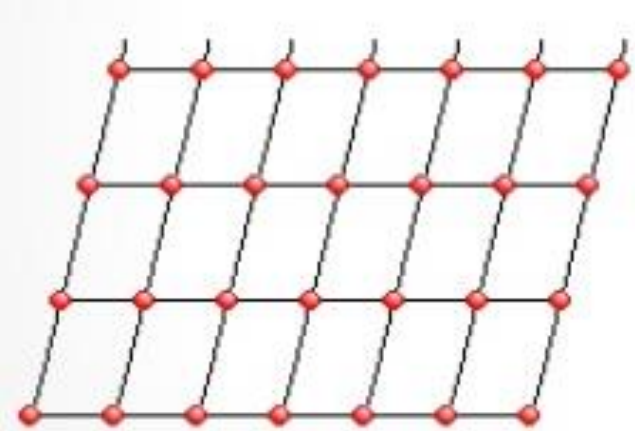
Crystal Lattice

Bravais Lattice

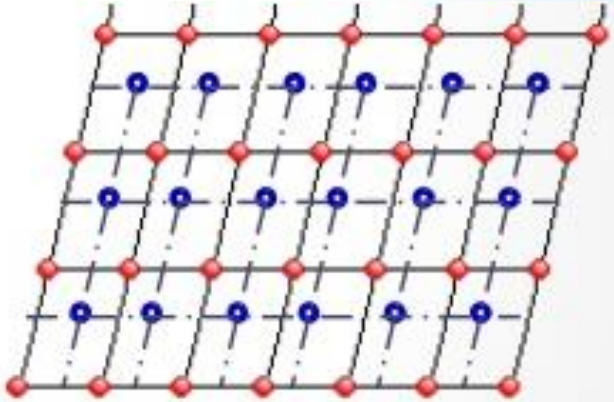
- All lattice points are equivalent
- All atoms in the crystal are of the same kind

Non-Bravais Lattice

- Some of the lattice points are not equivalent
- Atoms in the crystal are of the different kind
- Combination of 2 or more Bravais lattiice



Bravais Lattice

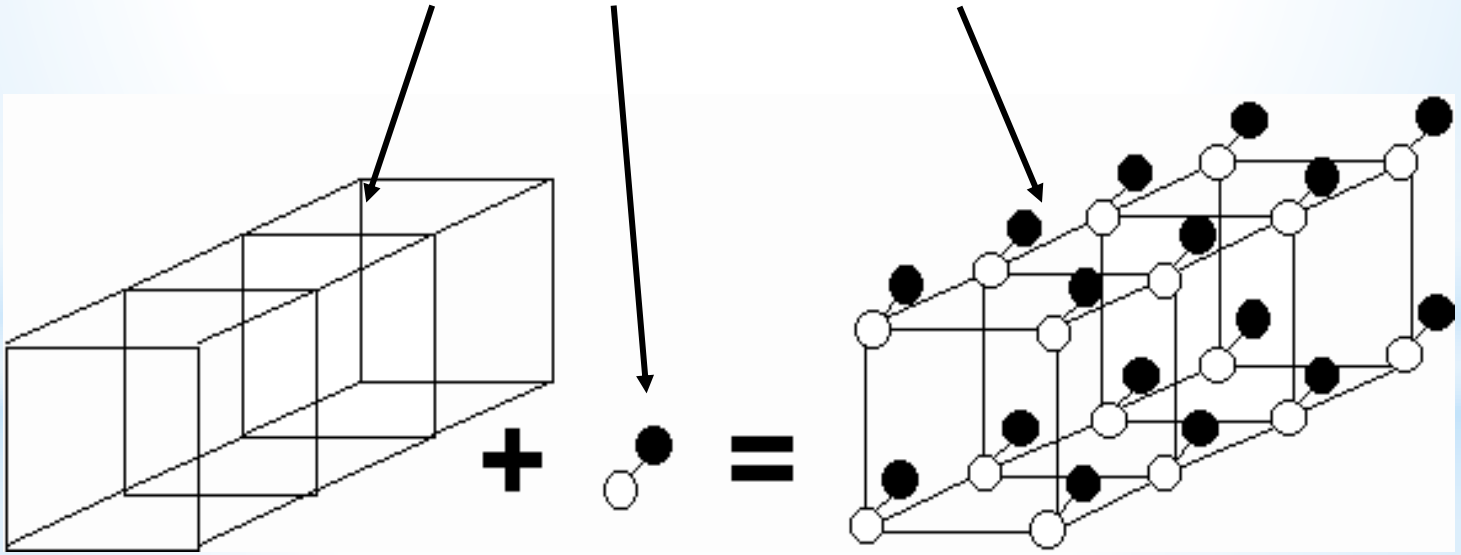


Non-Bravais Lattice

Basis: A crystal structure is formed when a group of atoms or molecules are attached identically to each lattice point. This group of atoms or molecules are called basis.

Basis is identical in composition, arrangement and orientation, which is repeated periodically in space to form the crystal structure.

Lattice + Basis = Crystal structure

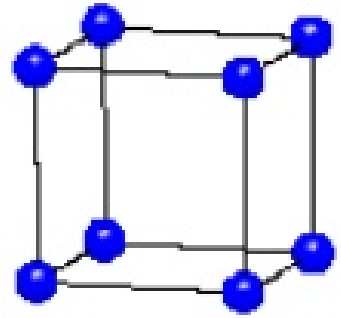


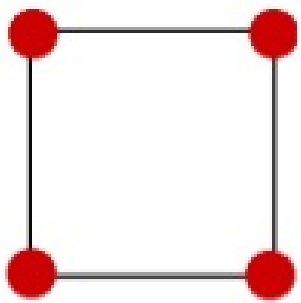
Unit cell

The smallest structural unit or building block that describes the crystal structure is called a unit cell of that structure.

Primitive cell

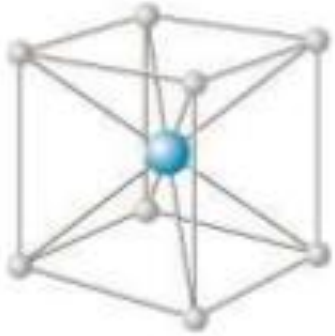
The minimum volume unit cell that can hold only one lattice point.

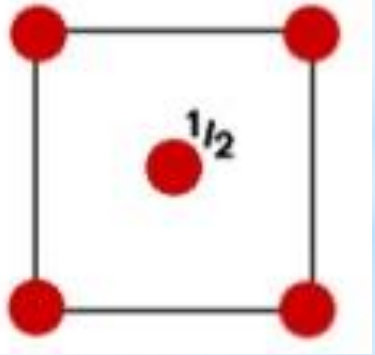


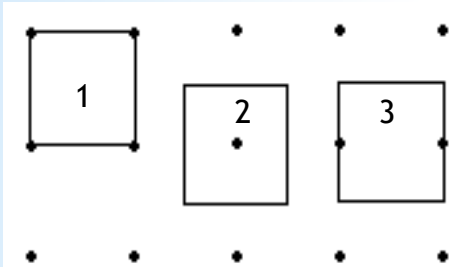


Non-primitive/ conventional cell

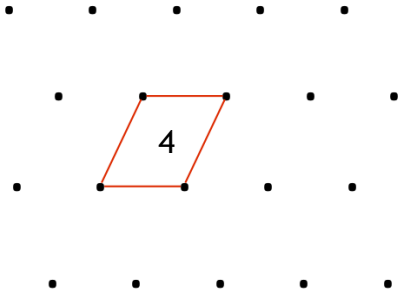
The minimum volume unit cell that can hold more than one lattice point.

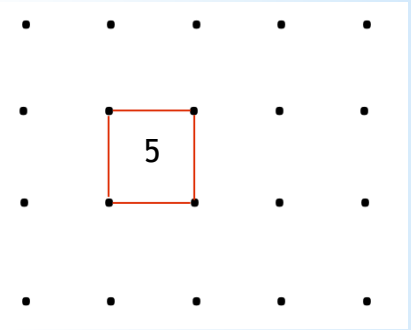


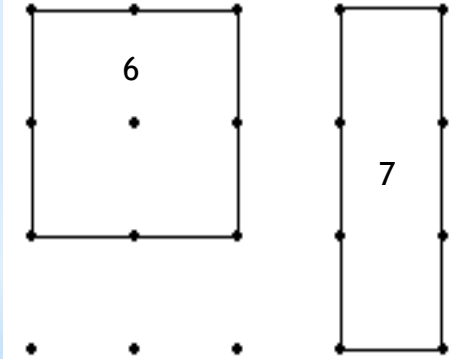




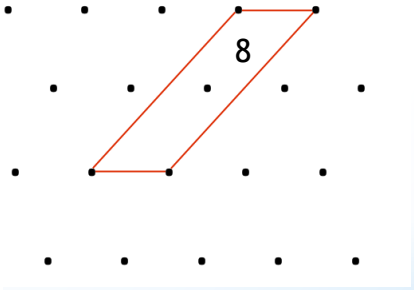
Primitive unit cells

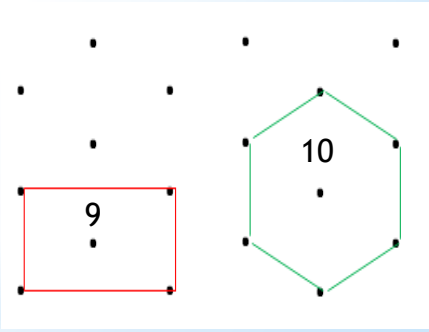






Non-primitive unit cells

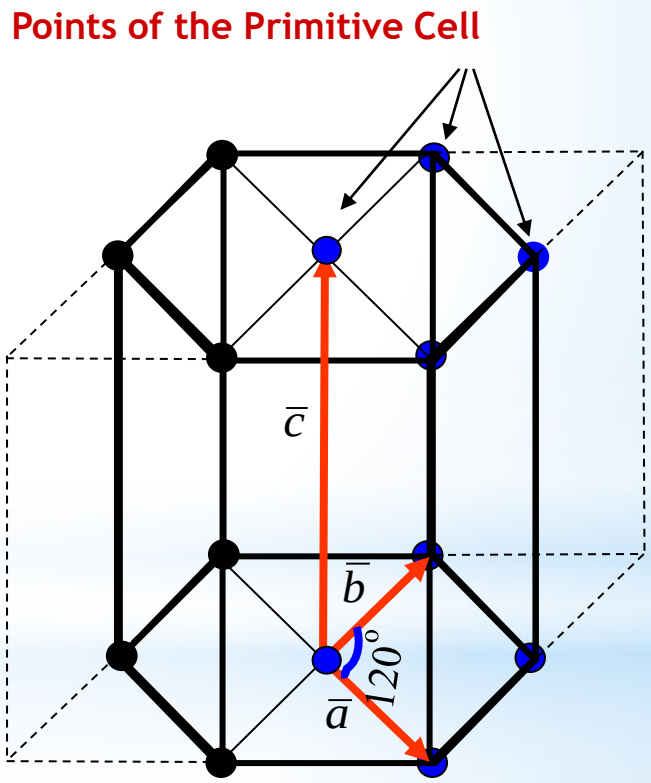




Conventional unit cell

A **conventional unit cell** of a lattice is one that contains the same point group symmetries as the overall lattice and is the smallest such **cell**.

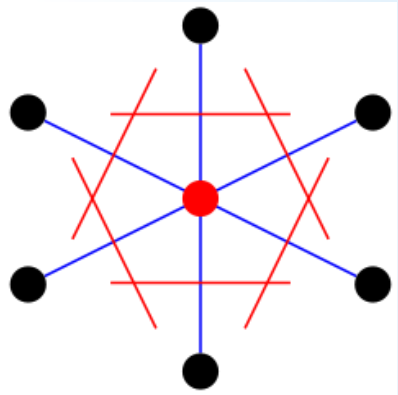
- Its basis vector defines a right-handed axial setting.
- Its edges are along symmetry direction of the lattice.
- It is the smallest cell compatible with the above conditions.
- Crystal having the same type of conventional cell belong to the same crystal family.

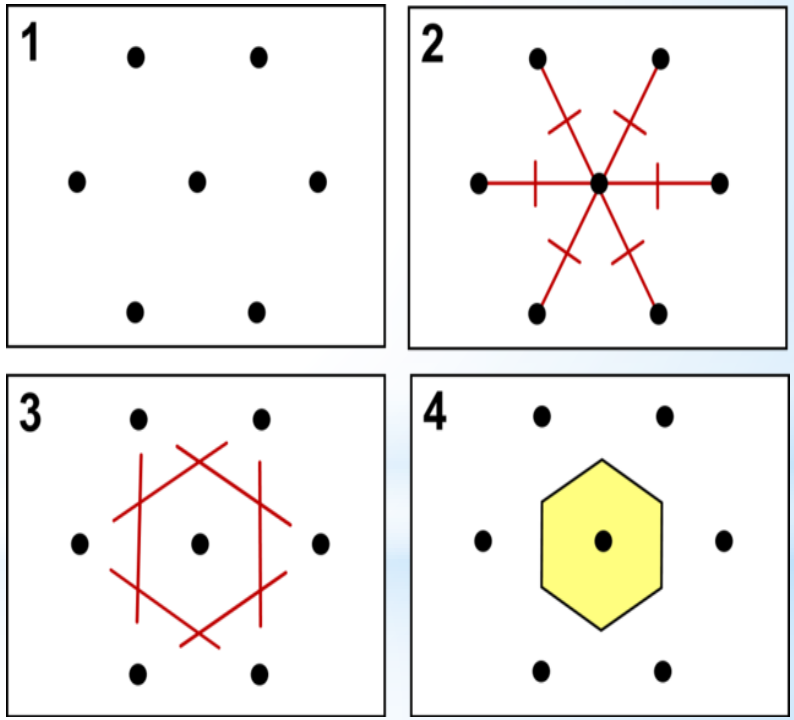


Wigner-Seitz cell

It was first suggested by E. P Wigner and F. Seitz. A primitive cell can also be chosen as:

1. Draw lines to connect a given lattice point to all nearby lattice points.
2. At the midpoint and normal to these lines draw new lines or planes.
3. The smallest volume enclosed in this way is the Wigner-Seitz primitive cell.





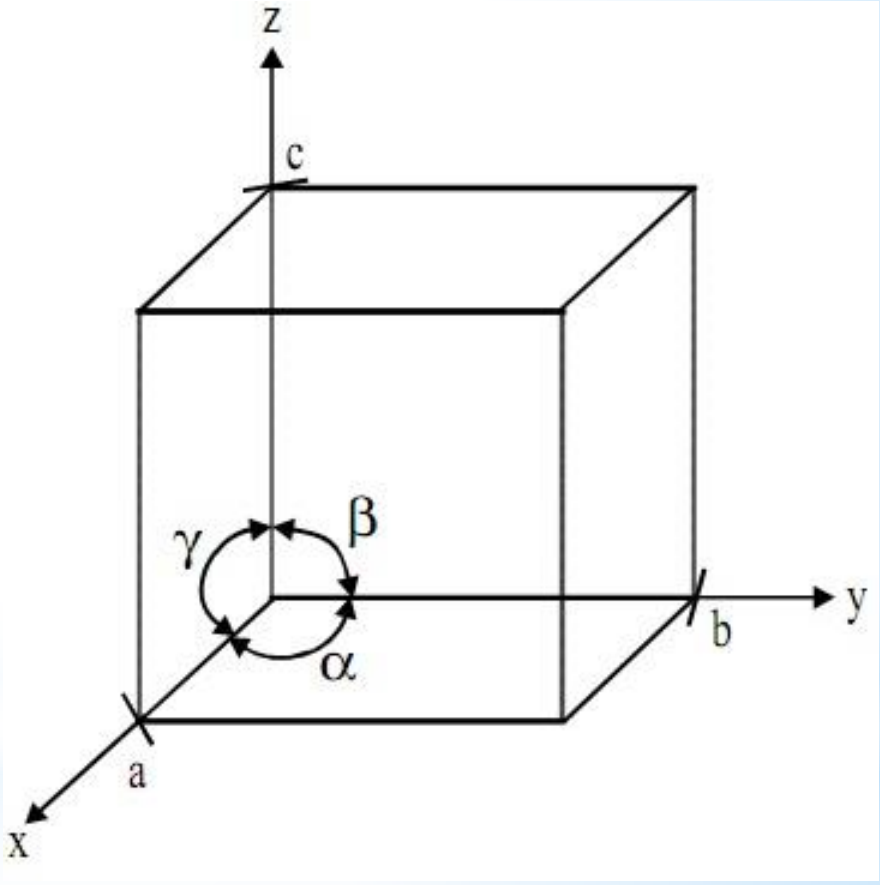
Lattice parameters

The parameters that are used to describe the size and the shape of a unit cell of a crystal lattice are known as the lattice parameters.

The magnitudes of 3 fundamental translation vectors (a, b and c) along with opposite angles (α, β, γ) each of between two crystallographic axis as shown in figure are the lattice parameters.

The distance between two identical atoms or molecules is the **lattice constant** (a, b, c).

a, b, c $\rightarrow$ describes the size and α, β, $\gamma\rightarrow$ describes the shape of the unit cell.

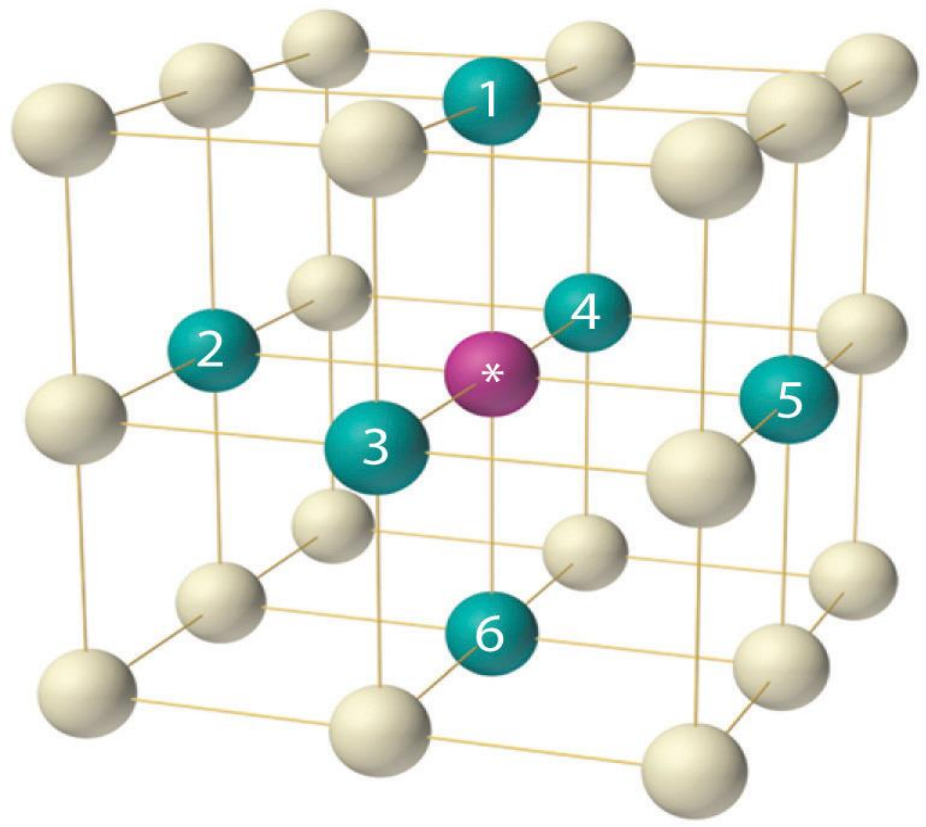


Co-ordination number

The points in a Bravais lattice that are closest to a given point are called its nearest neighbors. Because of the periodic nature of a Bravais lattice, each point has the same number of nearest neighbors. This number is thus a property of the lattice and is referred to as the coordination number of the lattice.

For an atom in the interior of a crystal lattice the number of atoms touching the given atom is the **bulk coordination number**; for an atom at a surface of a crystal, this is the **surface coordination number**.

Bulk coordination number> Surface coordination number

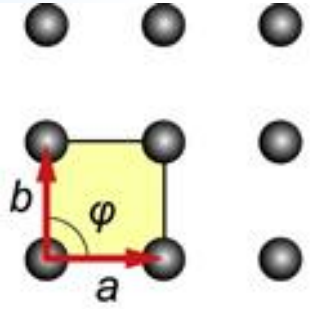


Co-ordination number of Simple Cubic Structure is 6

Two Dimensional Bravais Lattices

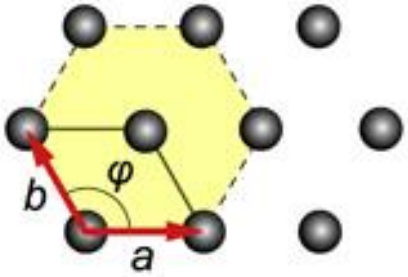
Lattice parameters are a,b and ϕ

5 distinct types of lattices.



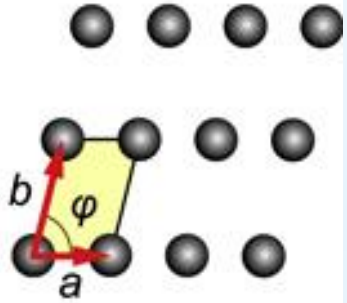
$|a| = |b|, \varphi = 90°$

Square



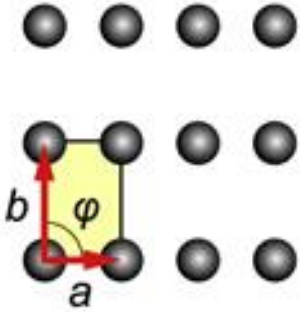
$|a| = |b|, \varphi = 120°$

Hexagonal



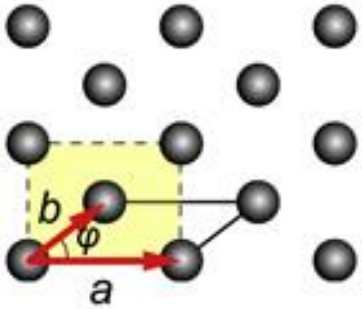
$|a| \neq |b|, \varphi \neq 90°$

Oblique



$|a| \neq |b|, \varphi = 90°$

Rectangular



$|a| \neq |b|, \varphi \neq 90°$

Centerd Rectangular