Primitive Lattice Cell

By

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Depending upon the arrangement of atoms or molecules, the solid may be classified as crystalline and non – crystalline solid.

1. Crystalline Solids (Long Range Order): The crystalline state of solid is characterized by regular and periodic arrangement of atoms or molecules. Most of the solids are crystalline in nature due to the fact that energy released during the formation of an ordered structure is more than that released during the formation of a disordered structure. Thus crystalline state is a low energy state and is therefore preferred by most of the solids. The crystalline solid may be sub-divided into single crystal and polycrystalline solids –

(a) Single Crystal Solid: In single crystals, the periodicity of the atoms extends throughout the material e.g. diamond, mica, quartz etc.

(b) Polycrystalline Solid: A polycrystalline solid is an arrangement of number of small crystallites with random orientations separated by well-defined boundaries. The small crystallites are known as *grains* and boundaries as *grain boundaries*. e.g. metals and ceramics.

2. Amorphous Solids(Short Range Order): The non – crystalline or amorphous solids are characterized by the complete random arrangement of atoms and molecules. e.g. glass, plastic, rubber etc.

Characteristics of Crystalline Solids:

i. The atoms and molecules are arranged in a definite order, giving them a definite geometrical form.

ii. The atoms are arranged in a long range order.

iii. All the bonds in atoms or molecules are equally strong.

Characteristics of Amorphous Solids:

i. The atoms and molecules are arranged in an irregular way.

ii. The atoms are arranged in a short range order.

iii. The chemical bonds between different atoms or molecules may not be equal.

Crystallography: The science which deals with the study of geometric forms and physical properties of crystalline solids is called *Crystallography*.

Crystal Lattice:A crystal lattice is a purely geometrical conception, consisting of points in space such that when the atoms (or group of atoms) which constitutes the crystal are placed on these points, we get the actual crystal.

Space Lattice: An arrangement of infinite number of points in 3 – D space with each point having **identical surroundings** is known as *Point Lattice* or *Space Lattice*.

The term **identical surroundings** means that lattice has the same appearance when viewed from a point $\vec{r}$ and from any other point $\vec{r}'$ in the lattice w.r.t. some arbitrary origin. This is possible only if the lattice contains a small group of point, called pattern unit which repeat itself in all directions by means of a translational operation $\vec{T}$ given by –

$$\vec{T} = n_1\vec{a} + n_2\vec{b} + n_3\vec{c} \qquad \text{---------- (1)}$$

where n_1, n_2, n_3 are arbitrary integers and the vectors $\vec{a}, \vec{b}, \vec{c}$ are called fundamental 'Translational Vectors' or 'Crystal Axes' or 'Basis Vectors'. Thus we have – $\vec{r}' = \vec{r} + \vec{T}$

OR $\vec{r}' = \vec{r} + n_1\vec{a} + n_2\vec{b} + n_3\vec{c}$ ---------- (2)

Those translational vectors which produces a translation operation containing integral coefficients (i.e. n_1, n_2, n_3 etc. are integral no.) are called 'Primitive Translation Vectors'.

Unit Cell:

A unit cell may also be defined as the smallest unit of lattice which on continuous repetition generates the complete lattice.

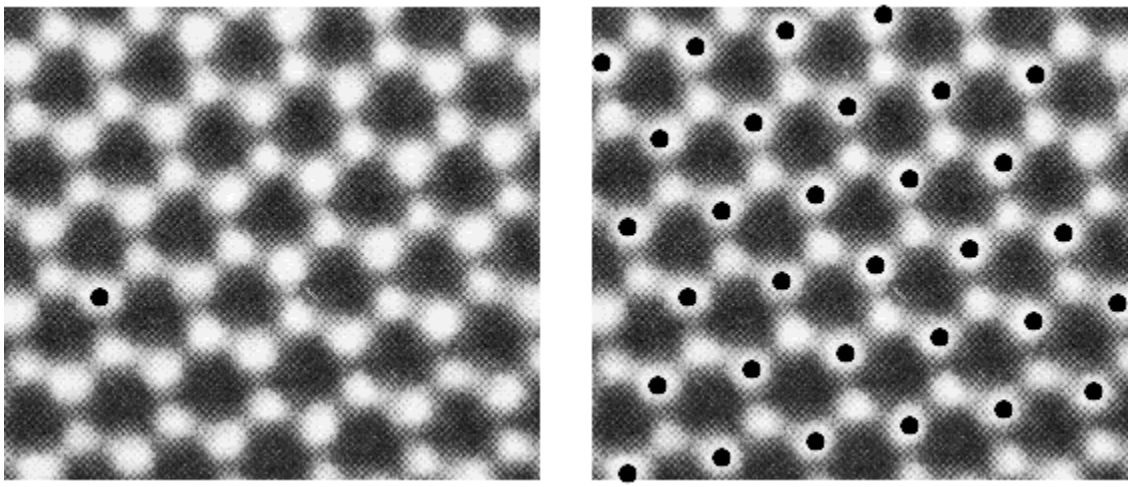
Primitive Cell

A **primitive cell** is a unit cell that contains exactly one lattice point. It is the smallest possible cell. If there is a lattice point at the edge of a cell and thus shared with another cell, it is only counted half. Accordingly, a point located on the corner of a cube is shared by 8 cubes and would count with 1/8.

Lattices

Crystalline structures are characterised by a repeating pattern in three dimensions. The periodic nature of the structure can be represented using a lattice.

To generate the lattice from any repeating pattern, we choose an arbitrary reference point and examine its environment. We then simply mark in all the points in the pattern that are identical to the chosen reference point. The set of identical points is the lattice, and each point within it is a **lattice point**.



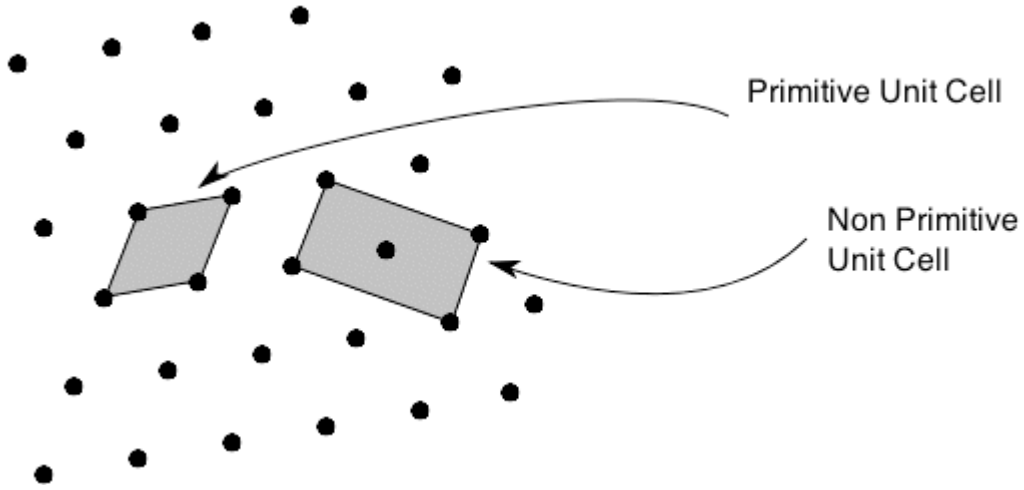
A. Putnis, *Introduction to Mineral Sciences*, Cambridge University Press, 1992

Note that not all white discs within this pattern are exactly equivalent, and therefore they are not all lattice points. The discs marked with a black spot have different arrangements around them than those that are unmarked (each is surrounded by 3 others in a triangle, but the orientation of the triangles is different).

Unit Cell

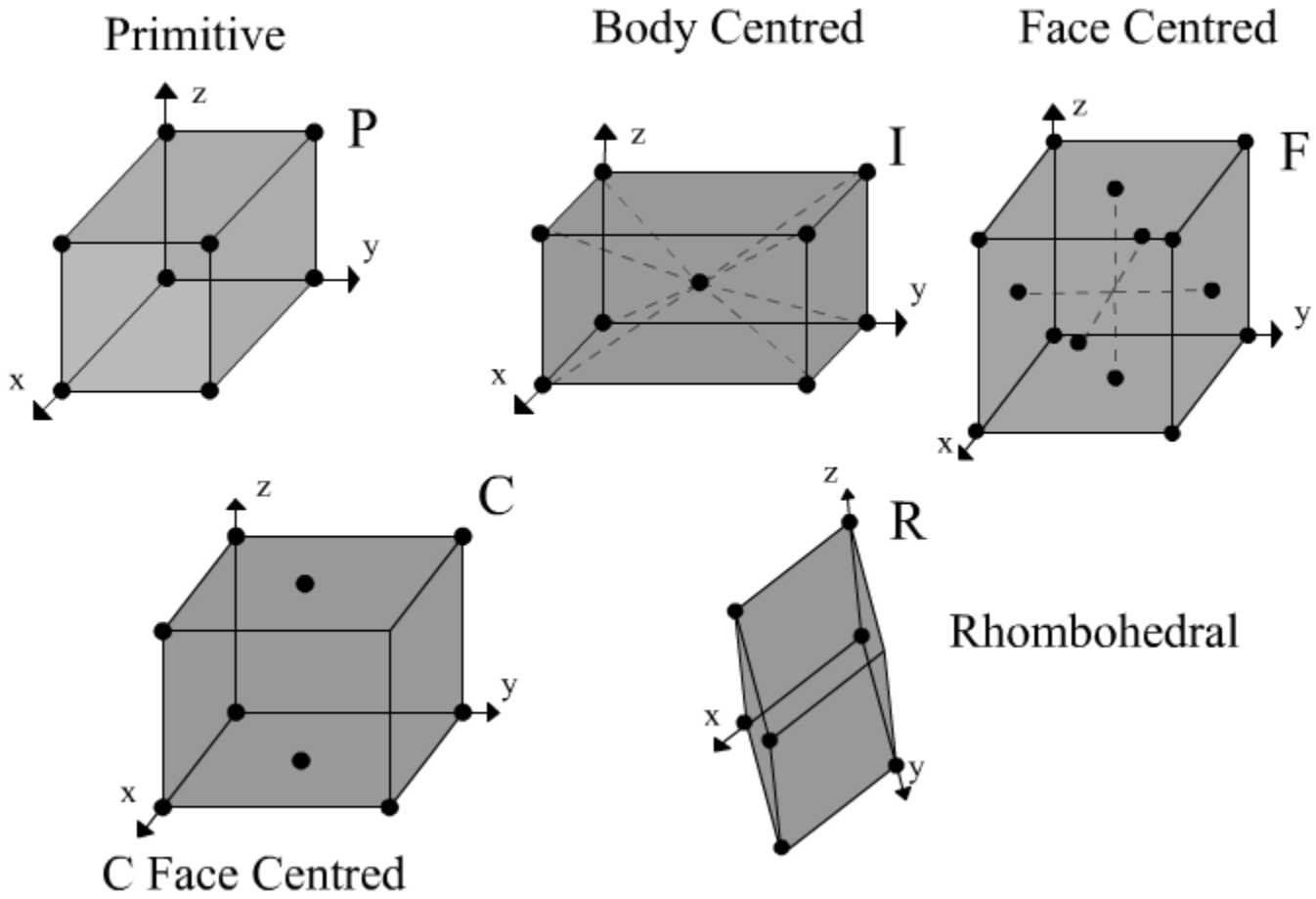
The structure of a crystal can be seen to be composed of a repeated element in three dimensions. This repeated element is known as the **unit cell**. It is the building block of the crystal structure. We define the unit cell in terms of the lattice (set of identical points). In three dimensions the unit cell is any parallelepiped whose vertices are lattice points, in two dimensions it is any parallelogram whose vertices are lattice points.

Of course this definition means that there are an infinite number of possible unit cells. So, in general, the unit cell is chosen such that it is the smallest unit cell that reflects the symmetry of the structure. There are two distinct types of unit cell: **primitive** and **non-primitive**. Primitive unit cells contain only one lattice point, which is made up from the lattice points at each of the corners. Non-primitive unit cells contain additional lattice points, either on a face of the unit cell or within the unit cell, and so have more than one lattice point per unit cell.



It is often the case that a primitive unit cell will not reflect the symmetry of the crystal structure. A suitable non-primitive unit cell will be picked in such cases.

The most common types of unit cell are the **primitive**(P) unit cell with one lattice point per unit cell; the **face centred**(F) unit cell with additional lattice points **at the centre of each face** and four lattice points per unit cell; and the **body centred**(I) unit cell with a lattice point in the middle of the unit cell and two lattice points per unit cell. Other cell types are the C face centred unit cell and the rhombohedral unit cell.



Lattice and Unit Cell Parameters

A lattice may be specified by two non-coincident vectors in 2D, and by three non-coplanar vectors in 3D. The vectors lie along the edges of the unit cell, and are labeled *a*, *b*, and (in 3D) *c*. The magnitude of the vectors is given by the dimensions of the unit cell in the real crystal under study.

The faces of the unit cell are labeled as follows:

- *A* : edges defined by lattice vectors *b* and *c*
- *B* : edges defined by lattice vectors *a* and *c*
- *C* : edges defined by lattice vectors *a* and *b*

Similarly, the *inter-facial angles* of the unit cell are defined to be:

- *alpha* : angle between edges *b* and *c*
- *beta* : angle between edges *a* and *c*
- *gamma* : angle between edges *a* and *b*

Lattice Systems: the 14 Bravais Lattices

Lattices can be classified into "systems", each system being characterized by the shape of its associated unit cell. In three dimensions, the lattices are categorized into seven crystal lattice "systems". Within several of these, lattices supporting non-primitive unit cells can be defined. The classification scheme yields a total of 14 possible lattices (called *Bravais* lattices).

The lattice symbols used for classification are as follows:

- P : primitive
- B : end-centered on B-face (convention for Monoclinic systems)
- C : end-centered on C-face (convention for Orthorhombic systems)
- I : body-centered
- F : face-centered
- R : rhombohedral primitive

System	**# of lattices in**	**Lattice**

	system	**symbols**
Triclinic (Anorthic)	1	P
Monoclinic	2	P, B
Orthorhombic	4	P, C, I, F
Tetragonal	2	P, I
Isometric (Cubic)	3	P, I, F
Trigonal/Rhombohedral	1	P or R
Hexagonal	1	P

In two dimensions, there are only four possible unit cell shapes and two possible lattice symbols:

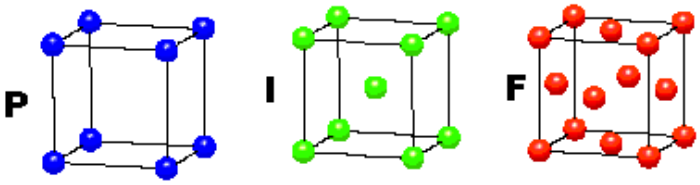
Cell shape	**Lattice symbol**
General parallelogram (rhomboid)	p

Rectangle	p, c
Square	p
Rhombus with 60 degree angle	p

CUBIC

$a = b = c$

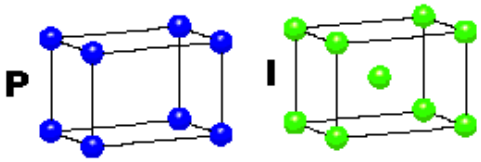
$\alpha = \beta = \gamma = 90°$



TETRAGONAL

$a = b \neq c$

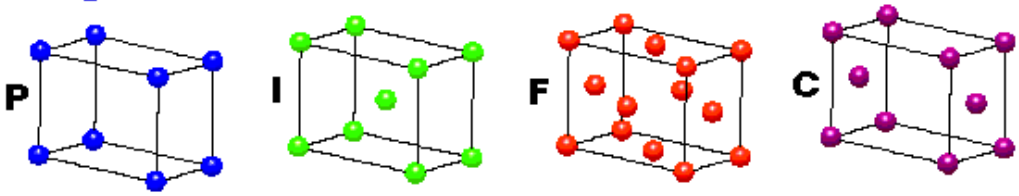
$\alpha = \beta = \gamma = 90°$



ORTHORHOMBIC

$a \neq b \neq c$

$\alpha = \beta = \gamma = 90°$

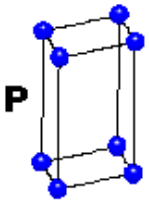


HEXAGONAL

$a = b \neq c$

$\alpha = \beta = 90°$

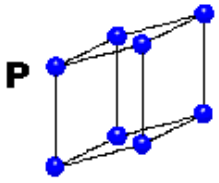
$\gamma = 120°$



TRIGONAL

$a = b = c$

$\alpha = \beta = \gamma \neq 90°$

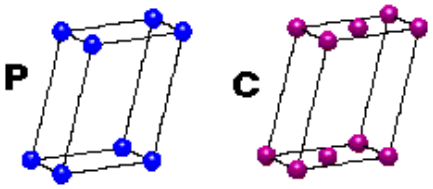


MONOCLINIC

$a \neq b \neq c$

$\alpha = \gamma = 90°$

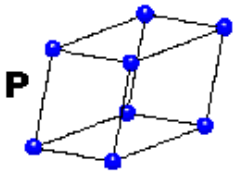
$\beta \neq 120°$



TRICLINIC

$a \neq b \neq c$

$\alpha \neq \beta \neq \gamma \neq 90°$



4 Types of Unit Cell
P = Primitive
I = Body-Centred
F = Face-Centred
C = Side-Centred
+
7 Crystal Classes
→ 14 Bravais Lattices