Crystal Structure

Unit Cell

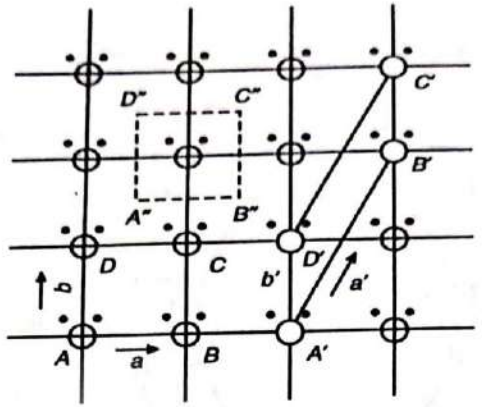


Fig. 1. A two-dimensional crystal lattice.

SOME CRYSTALLOGRAPHIC TERMS

If one replaces the atoms in a crystal by geometric points, one gets a regular periodic array of points. This array of points is called a *lattice*. The points are known as *lattice points*.

Figure 1 shows a two-dimensional crystal lattice. Here the parallelogram *ABCD* defined by the vectors $\vec{a}$ and $\vec{b}$ may be selected as a *unit cell* of the lattice. The vectors $\vec{a}$ and $\vec{b}$ are called the *basis vectors*. It is obvious from the figure that all translations of the *ABCD* parallelogram by integral multiples of the basis vectors $\vec{a}$ and $\vec{b}$ along the $\vec{a}$ and $\vec{b}$ directions will result in translating it to an exactly identical region in the crystal. Thus, the whole crystal may be reproduced merely by translating the area *ABCD* along the $\vec{a}$ and $\vec{b}$ directions by suitably multiplying the basis vectors $\vec{a}$ and $\vec{b}$. In other words, each lattice point in the crystal may be described by a vector $\vec{R}$ where $\vec{R} = h\vec{a} + k\vec{b}$; the constants h and k being integers. In some simple structures each lattice point is represented by only one atom whereas in others, a number of atoms forms a lattice point.

By extending the above procedure to *three dimensions* we define the following terms :

Unit Cell. This is a region of the crystal defined by the basis vectors $\vec{a}$, $\vec{b}$ and $\vec{c}$ such that a translation of this region by any integral multiple of these vectors will result in a similar region of the crystal.

Basis Vectors. Three linearly independent vectors $\vec{a}$, $\vec{b}$ and $\vec{c}$ used to define a unit cell are called the basis vectors.

Reciprocal Lattice

- The **reciprocal lattice**of a **reciprocal lattice** is the (original) direct **lattice**. The length of the **reciprocal lattice** vectors is proportional to the **reciprocal** of the length of the direct **lattice** vectors. This is where the term **reciprocal lattice** arises from.
- In the above figure (Figure-1), $\vec{a},\vec{b},\vec{c}$ etc are Reciprocal Lattice vectors.

Miller Indices:

- **Miller Indices** are a symbolic vector representation for the orientation of an atomic plane in a crystal lattice and are defined as the reciprocals of the fractional intercepts which the plane makes with the crystallographic axes.
- **Miller indices** form a notation system in crystallography for planes in crystal (Bravais) lattices.
- Miller indices are used to specify directions and planes.
- These directions and planes could be in lattices or in crystals.
- The number of indices will match with the dimension of the lattice or the crystal.
- E.g. in 1D there will be 1 index and 2D there will be two indices etc.

y
s a point – note the exclusive use

rs/directions are denoted with a bar on top of the

a direction
a family of directions
a plane
a family of planes

Miller Indices for Directions

- A vector r passing from the origin to a lattice

point can be written as:

r = r1 a + r2 b + r3c

where, a, b, c → basic vectors and

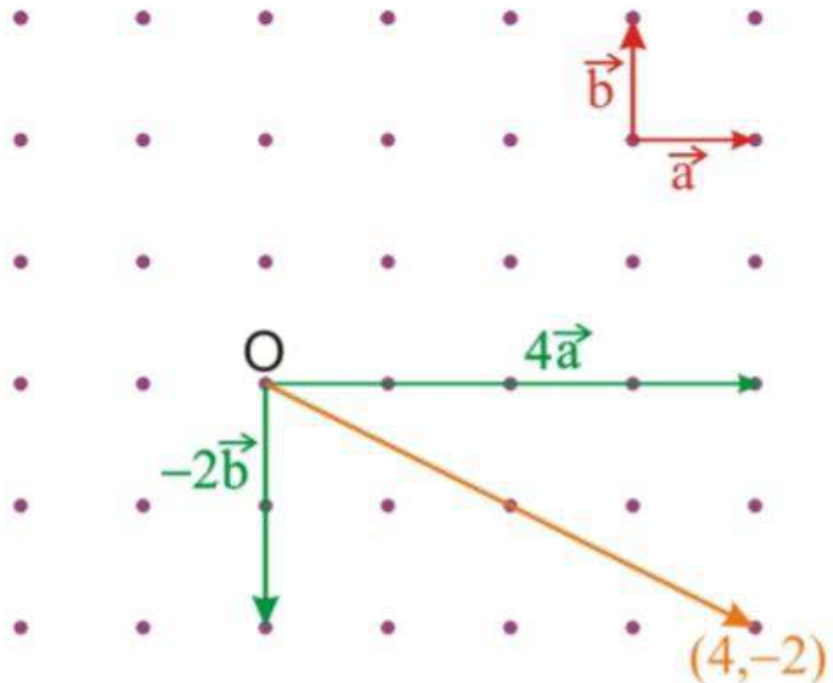
miller indices → (r1r2r3)

- Fractions in (r1r2r3) are eliminated by multiplying all components by

their common denominator.

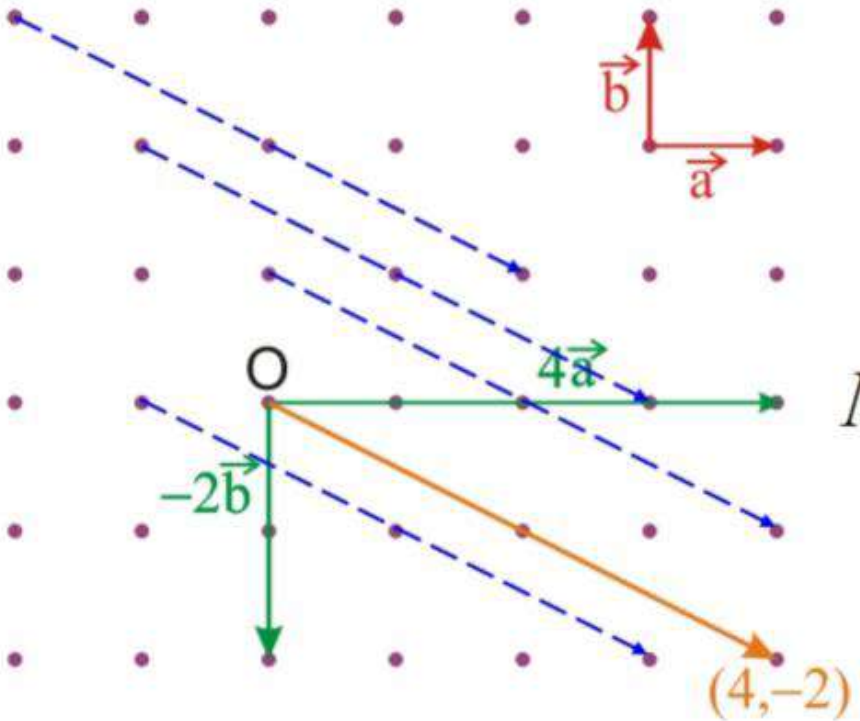
- [e.g. (1, ¾ ,½) will be expressed as (432)]

Example



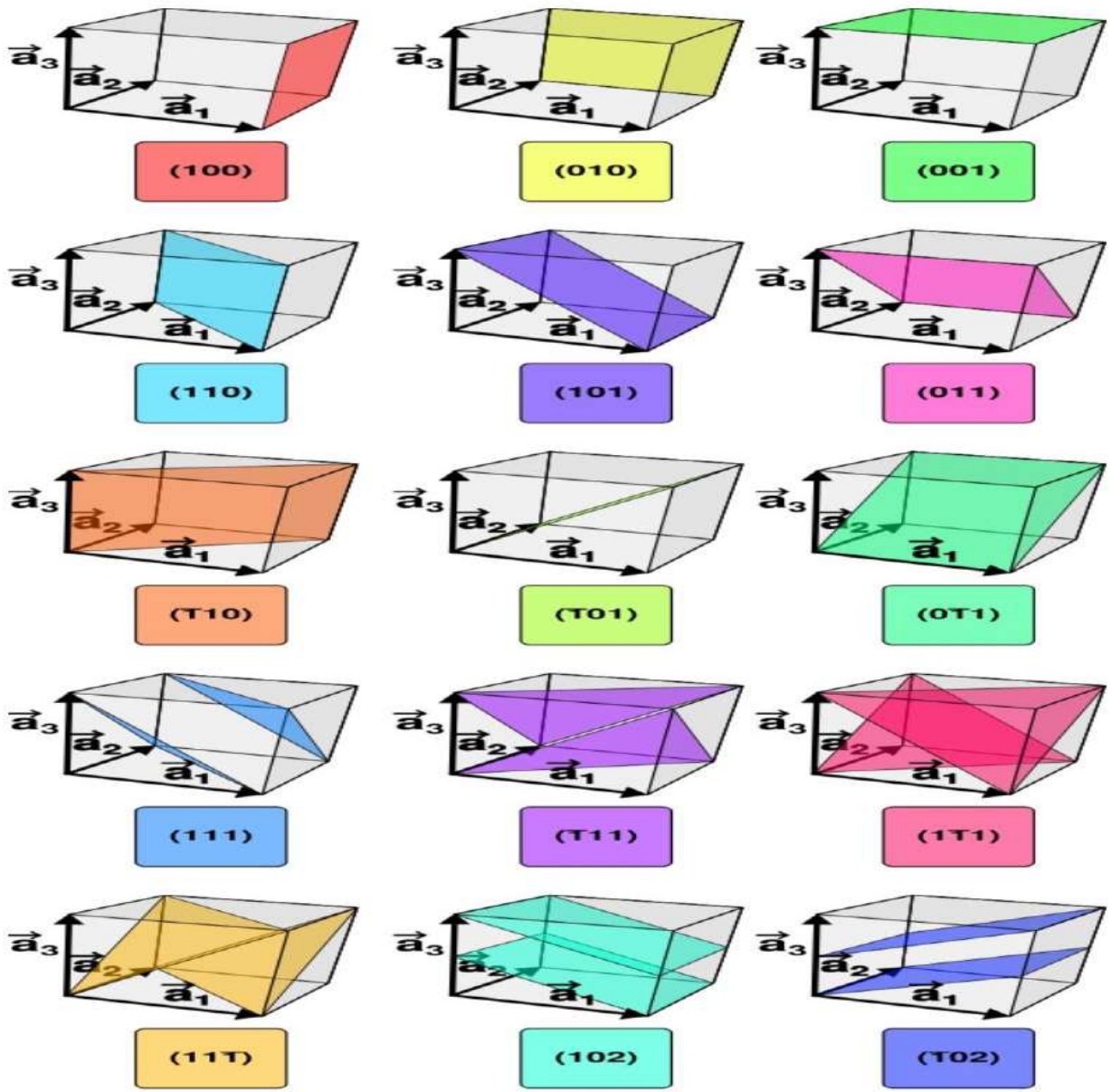
Miller Indices $\rightarrow [4\bar{2}]$

Example (cont'd)



Miller Indices → $[4\bar{2}]$

The index represents a set of all such parallel vectors



Planes with different Miller indices in cubic crystals

Bravais Lattice

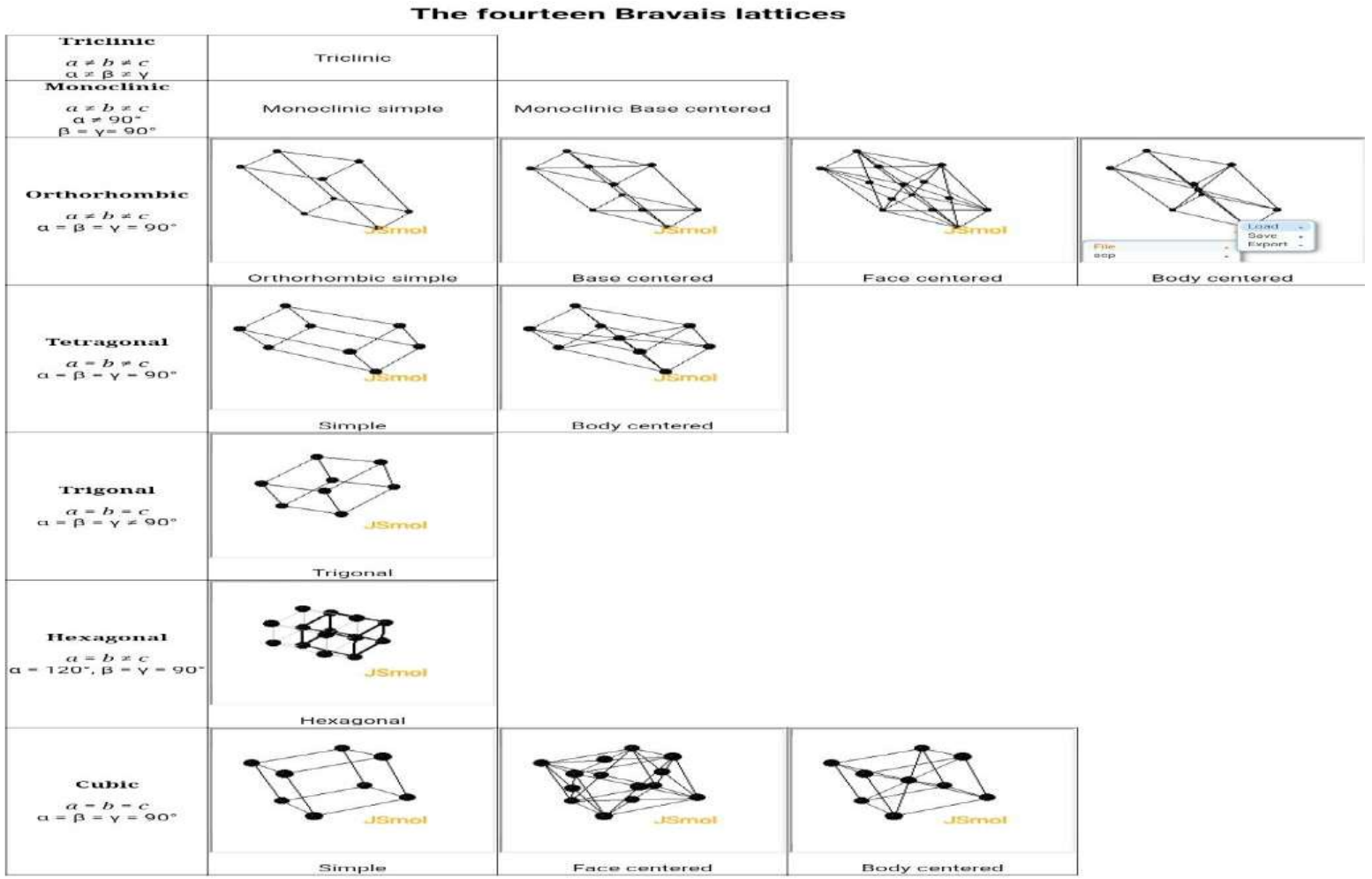
Bravais Lattice refers to the ***14 different 3-dimensional configurations into which atoms can be arranged in crystals.*** The smallest group of symmetrically aligned atoms which can be repeated in an array to make up the entire crystal is called a **unit cell**.

There are several ways to describe a lattice. The most fundamental description is known as the Bravais lattice. In words, a Bravais lattice is an array of discrete points with an arrangement and orientation that look exactly the same from any of the discrete points, that is the lattice points are indistinguishable from one another.

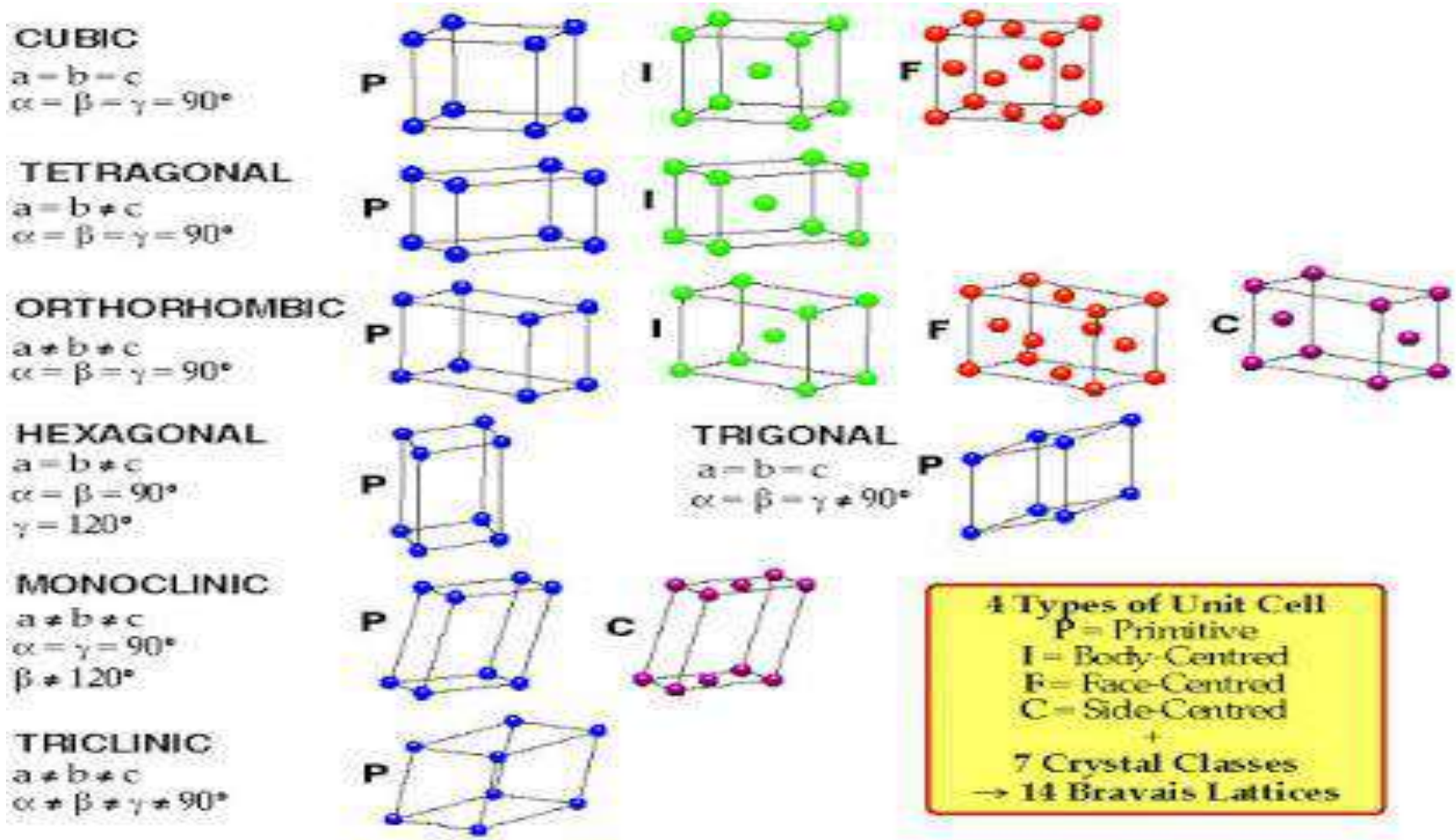
Thus, a Bravais lattice can refer to one of the 14 different types of unit cells that a crystal structure can be made up of. These lattices are **named after the French physicist Auguste Bravais.**

14 Types of Bravais Lattices

Out of 14 types of Bravais lattices some 7 types of Bravais lattices in three-dimensional space are listed in this subsection. Note that the letters a, b, and c have been used to denote the dimensions of the unit cells whereas the letters ***α, β, and γ*** denote the corresponding angles in the unit cells.



The 14 Bravais **lattices** are grouped into seven **lattice** systems: triclinic, monoclinic, orthorhombic, tetragonal, rhombohedral, hexagonal, and cubic. In a crystal system, a set of point groups and their corresponding space groups are assigned to a **lattice** system.



Brillouin Zone

The Brillouin zone is a very important concept in solid state physics; it plays a major role in the theoretical understanding of the elementary ideas of electronic energy bands. The first Brillouin zone is defined as the Wigner–Seitz primitive cell of the reciprocal lattice. Thus, it is the set of points in the reciprocal space that is closer to $K = 0$ than to any other reciprocal lattice point. We have shown in Figure 1.21 that the Bragg planes bisect the lines joining 0 (the origin) to the reciprocal lattice points. Thus, we can also define the first Brillouin zone as the set of points that can be reached from 0 without crossing any Bragg planes. Here, the points common to the surface of two or more zones have not been considered.

The second Brillouin zone is the set of points that can be reached from the first Brillouin zone by crossing only one plane. Similarly, the nth Brillouin zone can be defined as the set of points that can be reached by crossing $n - 1$ Bragg planes. We will first describe Brillouin zones of one- and two-dimensional (square) lattices to explain the fundamental methods of obtaining the Brillouin zones before describing the Brillouin zones of some important lattices.

Some youtube links

- https://youtu.be/KQYej8nanYk
- https://youtu.be/BjVTdZ_htu8
- https://youtu.be/DFFU39A3fPY
- https://youtu.be/wHmJdwqVk9g
- https://youtu.be/iyJvxOLq02s
- https://youtu.be/5Jw05CU0Nk8
- https://youtu.be/oLmjzSsO4Tw
- https://youtu.be/_jkXqzdJhp8
- https://youtu.be/QC8_Q5CnvBs
- https://youtu.be/_r_ZSS8absk
- https://youtu.be/qr1erveViHA
- https://youtu.be/61Lgo56bBbg

THANK YOU*