KATILARIN ELEKTRONİK YAPISININ BENZETİŞİMİ

Kristal Fiziği: Temel Kavramlar-1

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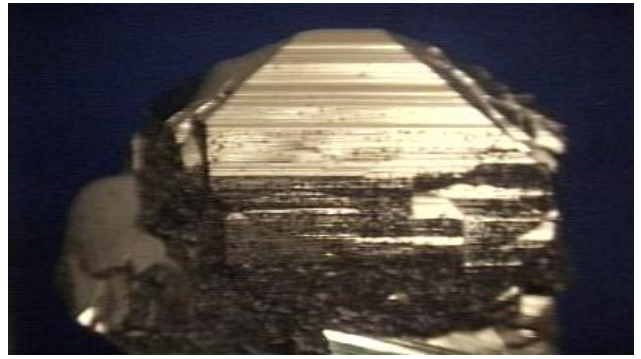
CRYSTALLOGRAPHY

What is crystallography?

The branch of science that deals with the geometric description of crystals and their internal arrangement.



Crystallography

Crystallography is essential for solid state physics

- **Symmetry of a crystal can have a profound influence on its properties.**
- **Any crystal structure should be specified completely, concisely and unambiguously.**
- **Structures should be classified into different types according to the symmetries they possess.**

ELEMENTARY CRYSTALLOGRAPHY

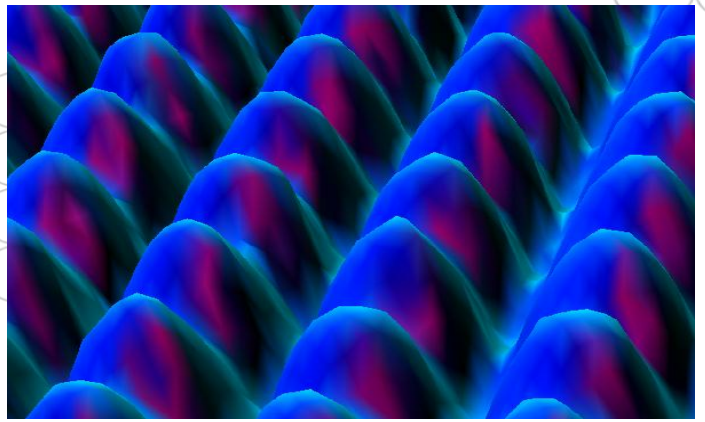
- **A basic knowledge of crystallography is essential for solid state physicists;**
  - **to specify any crystal structure and**
  - **to classify the solids into different types according to the symmetries they possess.**
- **Symmetry of a crystal can have a profound influence on its properties.**
- **We will concern in this course with solids with simple structures.**

CRYSTAL LATTICE

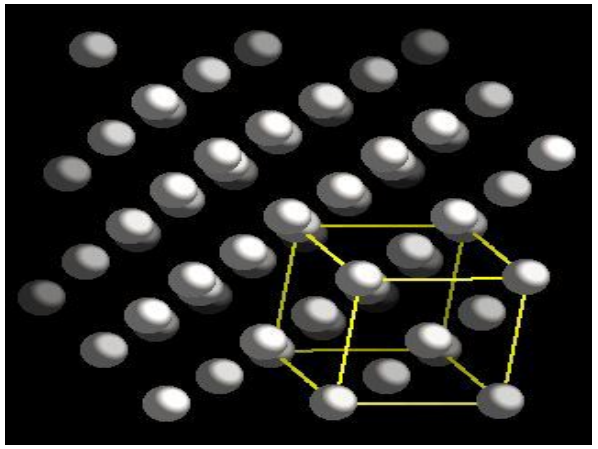
What is crystal (space) lattice?

In crystallography, only the geometrical properties of the crystal are of interest, therefore one replaces each atom by a geometrical point located at the equilibrium position of that atom.

Platinum



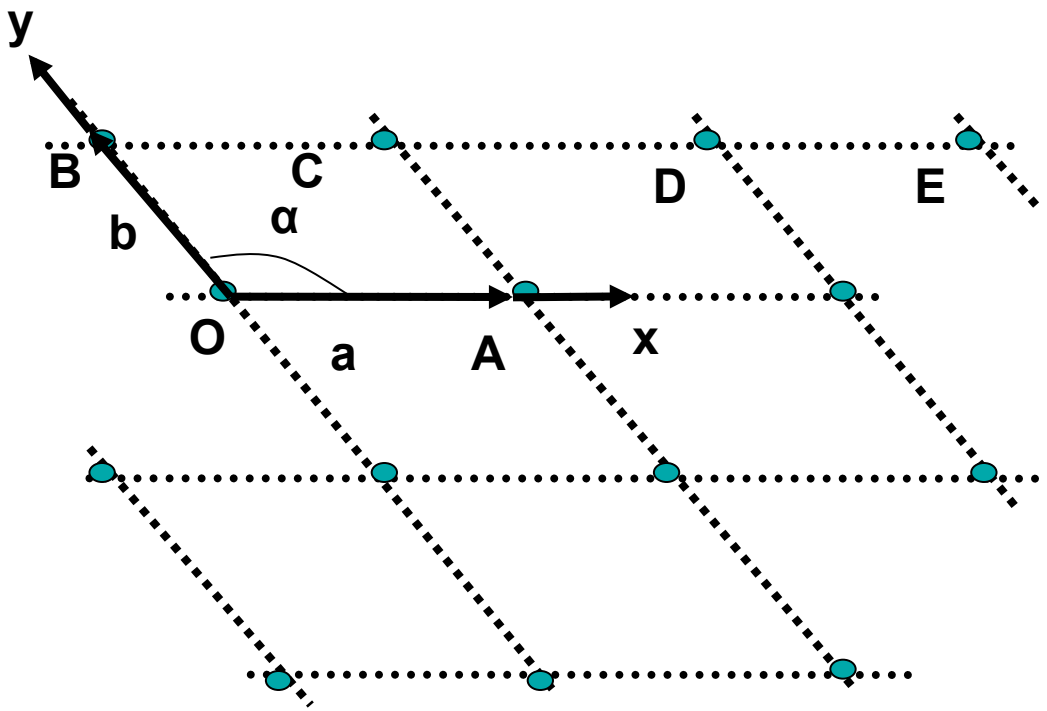
Platinum surface
(scanning tunneling microscope)



Crystal lattice and structure of Platinum

Crystal Lattice

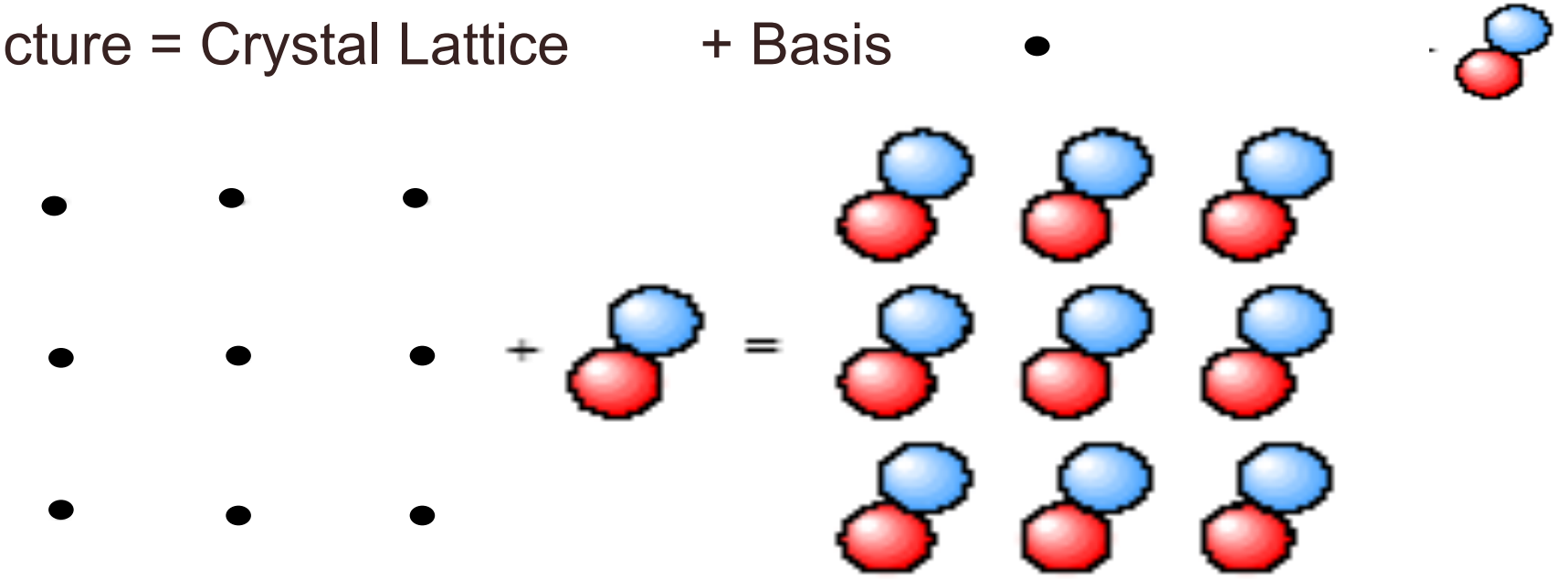
- **An infinite array of points in space,**
- **Each point has identical surroundings to all others.**
- **Arrays are arranged exactly in a periodic manner.**



Crystal Structure

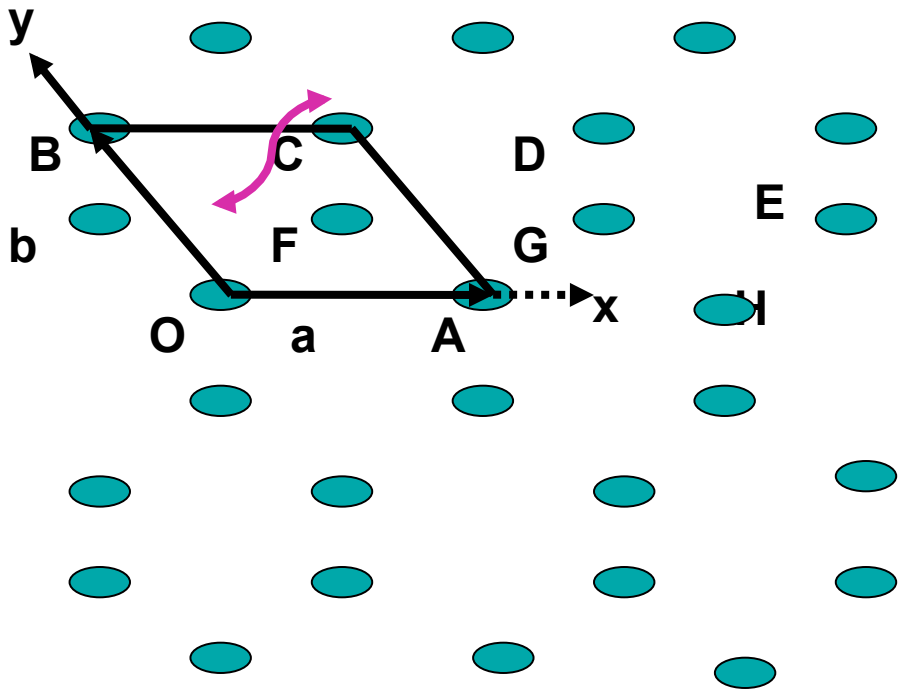
- **Crystal structure can be obtained by attaching atoms, groups of atoms or molecules which are called basis (motif) to the lattice sides of the lattice point.**

Crystal Structure = Crystal Lattice + Basis

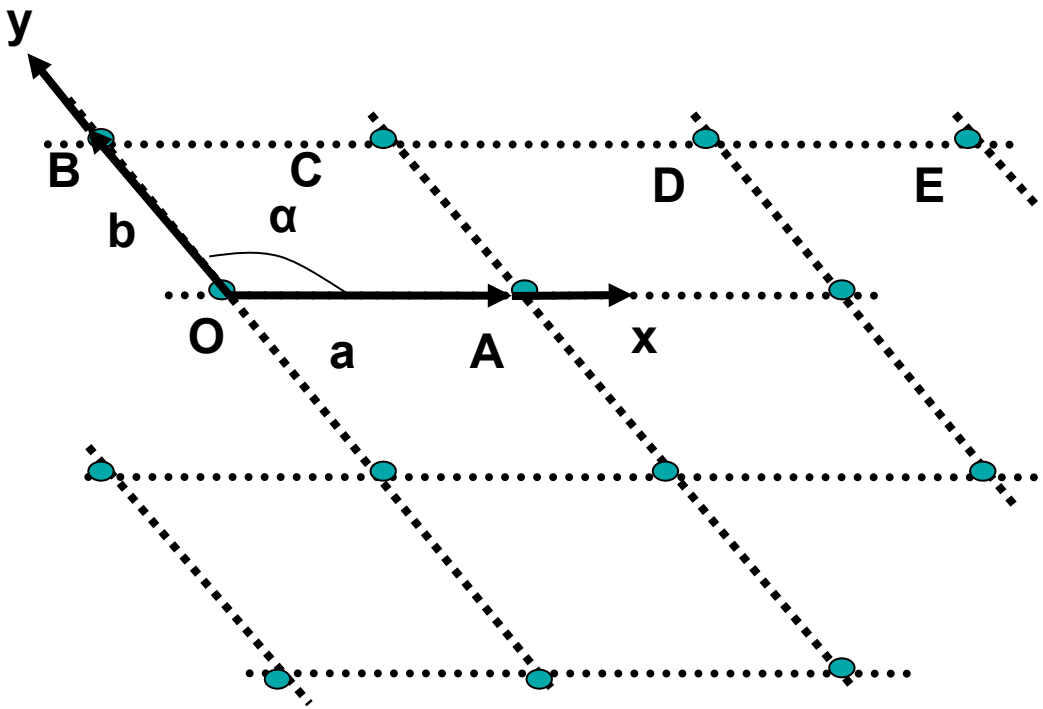


Basis

- A group of atoms which describe crystal structure



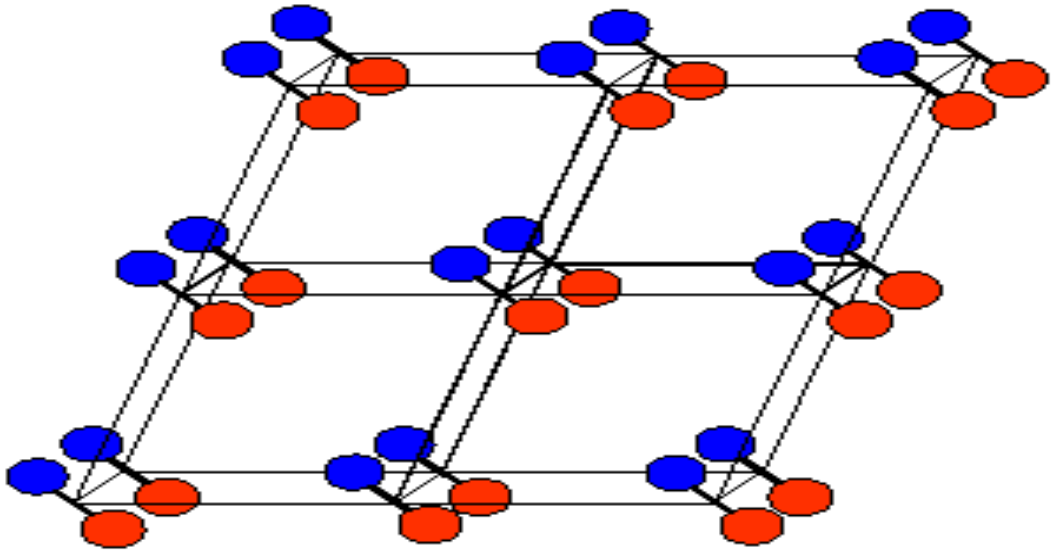
a) Situation of atoms at the corners of regular hexagons



b) Crystal lattice obtained by identifying all the atoms in (a)

Crystal structure

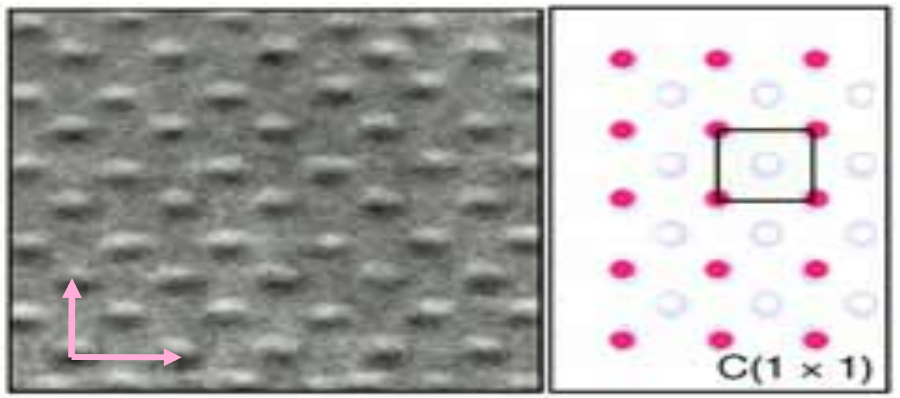
- **Don't mix up atoms with lattice points**
- **Lattice points are infinitesimal points in space**
- **Lattice points do not necessarily lie at the centre of atoms**



Crystal Structure = Crystal Lattice + Basis •

Types Of Crystal Lattices

1) Bravais lattice is an infinite array of discrete points with an arrangement and orientation that appears exactly the same, from whichever of the points the array is viewed. Lattice is invariant under a translation.



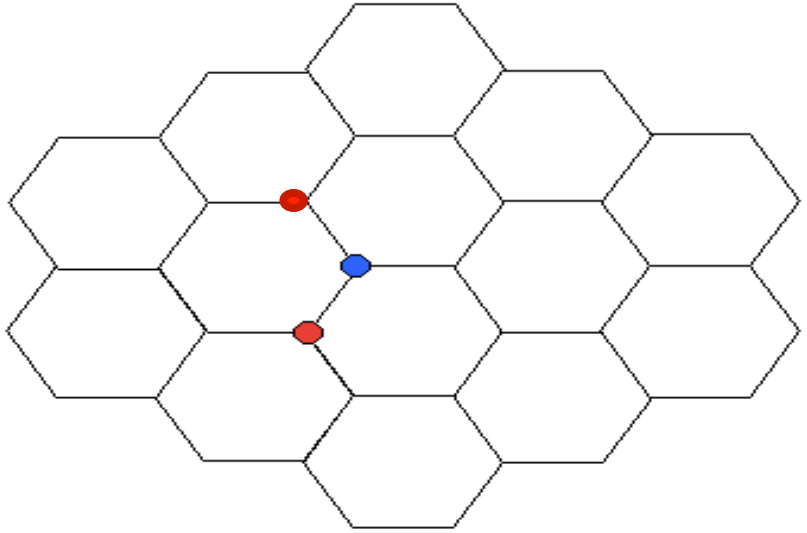
Nb film

Types Of Crystal Lattices

2) Non-Bravais Lattice

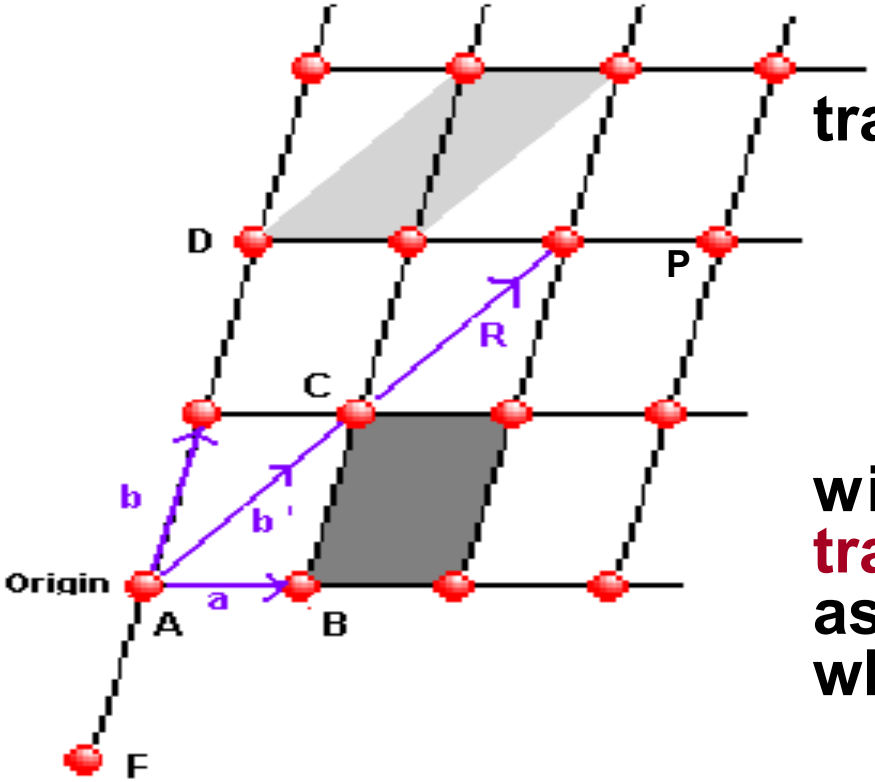
Not only the arrangement but also the orientation must appear exactly the same from every point in a bravais lattice.

- **The red side has a neighbour to its immediate left, the blue one instead has a neighbour to its right.**
- **Red (and blue) sides are equivalent and have the same appearance**
- **Red and blue sides are not equivalent. Same appearance can be obtained rotating blue side 180º.**



Honeycomb

Translational Lattice Vectors – 2D



Point D(n1, n2) = (0,2)

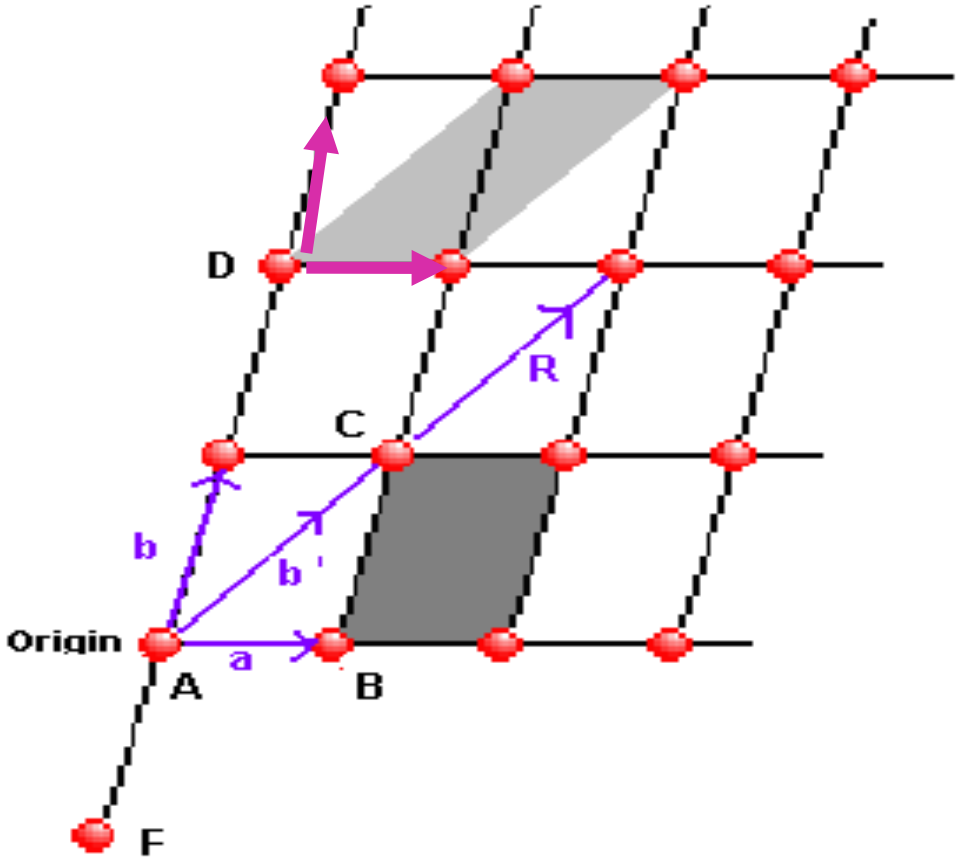
Point F (n1, n2) = (0,-1)

A space lattice is a set of points such that a translation from any point in the lattice by a vector;

$$R_n = n_1\, a + n_2\, b$$

locates an exactly *equivalent* point, *i.e.* a point with the same environment as *P* . This is translational symmetry. The vectors *a*, *b* are known as lattice vectors and (n_1, n_2) is a pair of integers whose values depend on the lattice point.

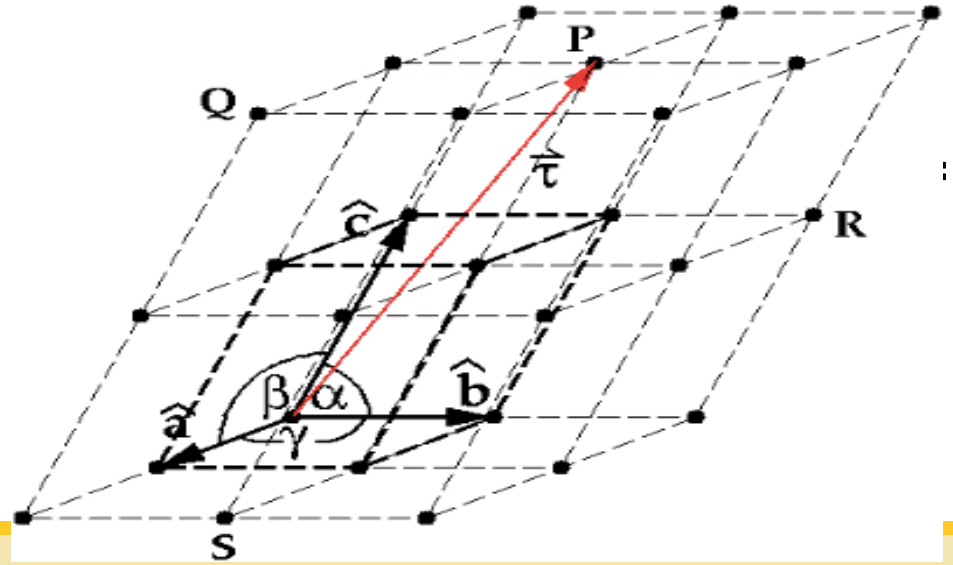
Lattice Vectors – 2D



- **The <u>two vectors a</u> and <u>b</u> form a set of lattice vectors for the lattice.**
- ***The choice of lattice vectors is not unique*. Thus one could equally well take the <u>vectors a and b' as a lattice vectors.</u>**

Lattice Vectors – 3D

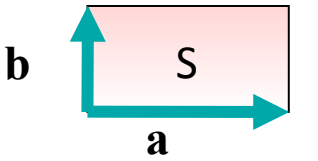
An ideal three dimensional crystal is described by 3 fundamental translation vectors a, b and c. If there is a lattice point represented by the position vector r, there is then also a lattice point represented by the position vector where *u*, *v* and *w* are arbitrary integers.



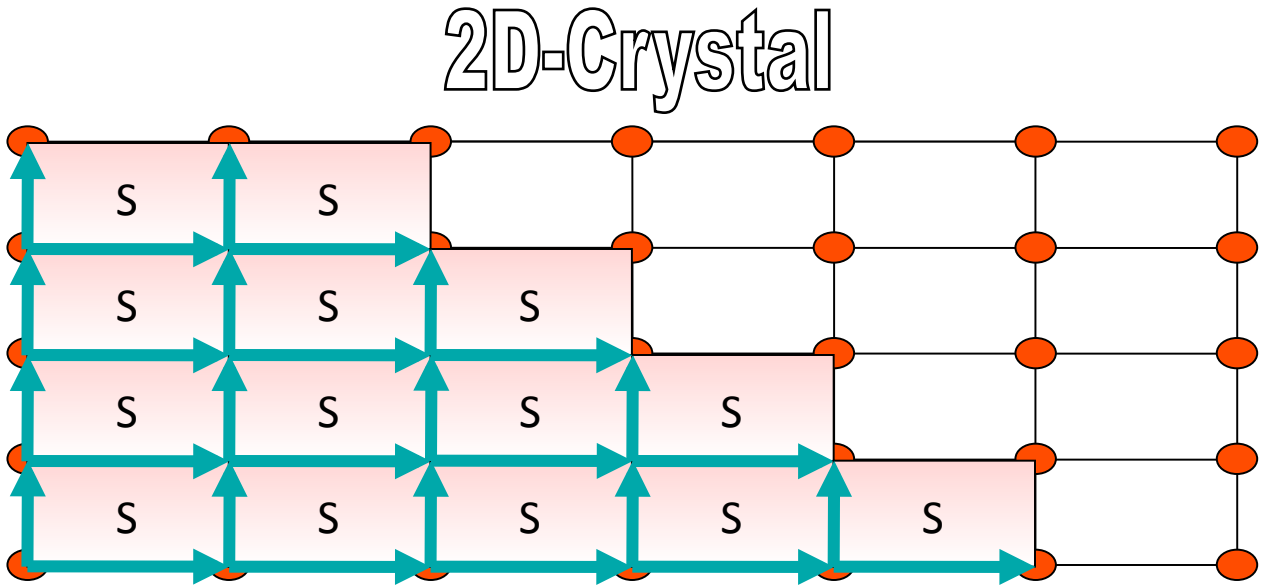
$$r + u\,a + v\,b + w\,c \qquad (1)$$

Unit Cell in 2D

- **The smallest component of the crystal (group of atoms, ions or molecules), which when stacked together with pure translational repetition reproduces the whole crystal.**



Unit Cell



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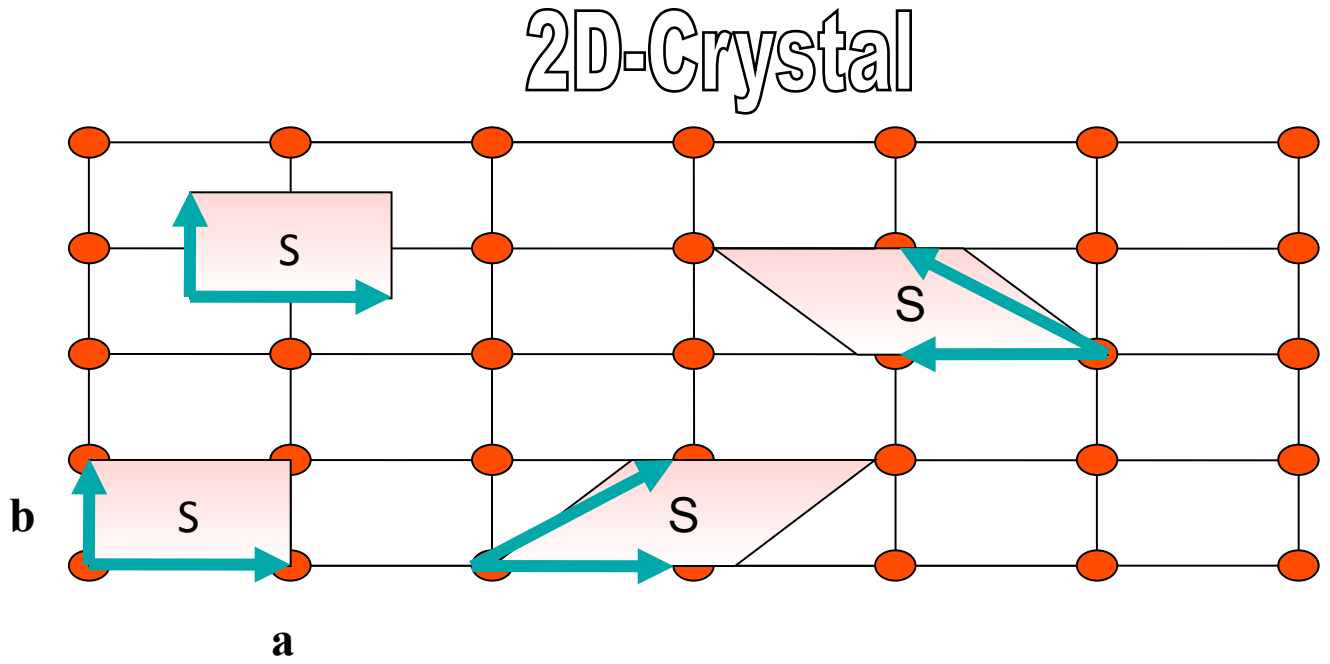
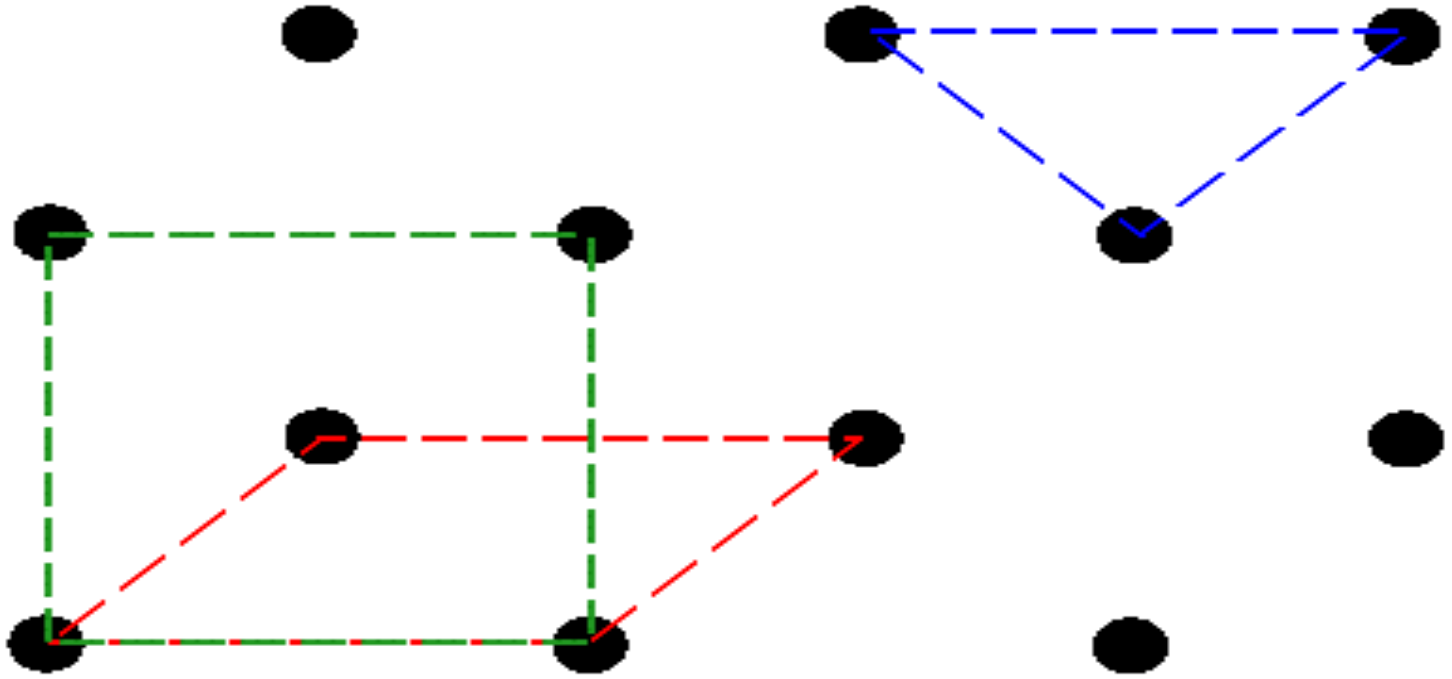
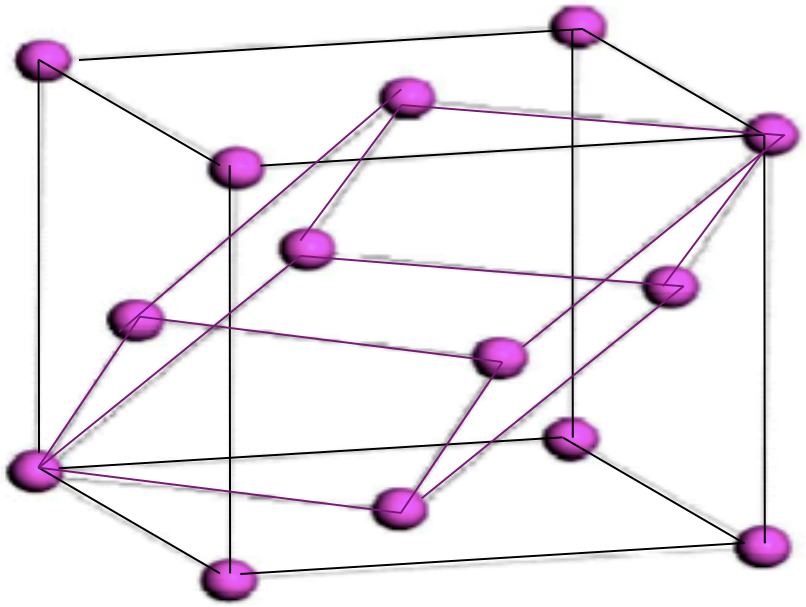


Why can't the blue triangle be a unit cell?



The Conventional Unit Cell

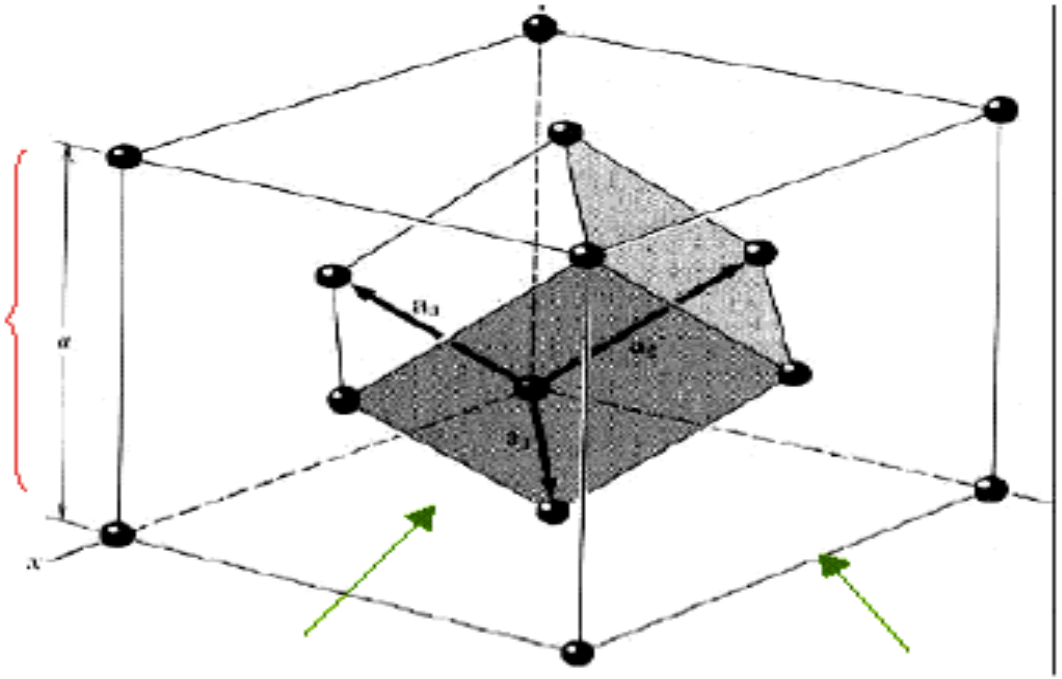


FCC Bravais lattice

- A unit cell just fills space when translated through a subset of Bravais lattice vectors.
- The conventional unit cell is chosen to be larger than the primitive cell, but with the full symmetry of the Bravais lattice.
- The size of the conventional cell is given by the lattice constant a.

Primitive and conventional cells of FCC

lattice constant



primitive vectors

$$\vec{a}_1 = \frac{a}{2}(\hat{x} + \hat{y}),$$

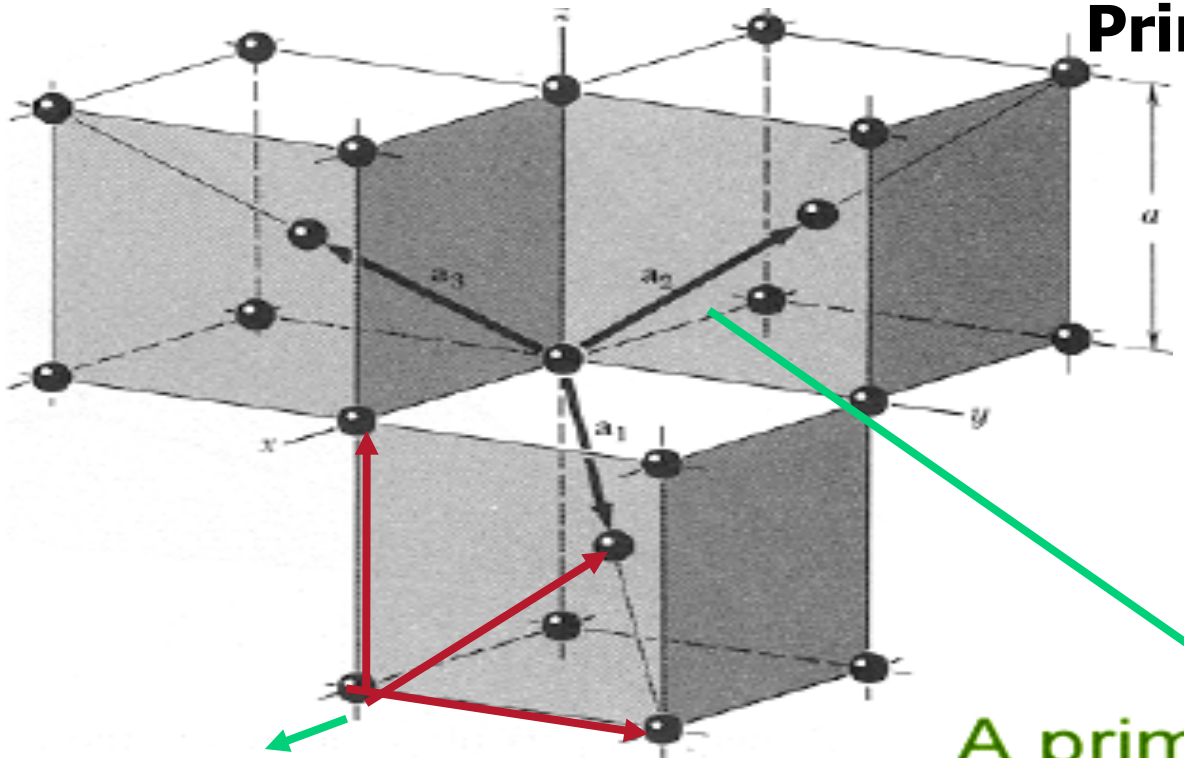
$$\vec{a}_2 = \frac{a}{2}(\hat{y} + \hat{z}),$$

$$\vec{a}_3 = \frac{a}{2}(\hat{z} + \hat{x}).$$

A primitive unit cell

a conventional unit cell

Primitive and conventional cells of BCC



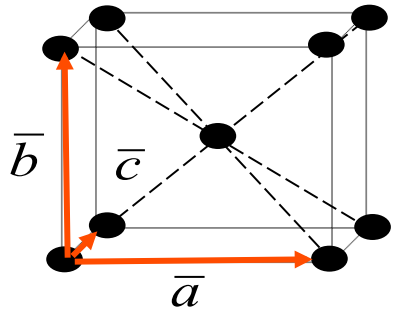
Primitive Translation Vectors:

$$\vec{a}_1 = \frac{1}{2}(\hat{x} + \hat{y} - \hat{z})$$

$$\vec{a}_2 = \frac{1}{2}(-\hat{x} + \hat{y} + \hat{z})$$

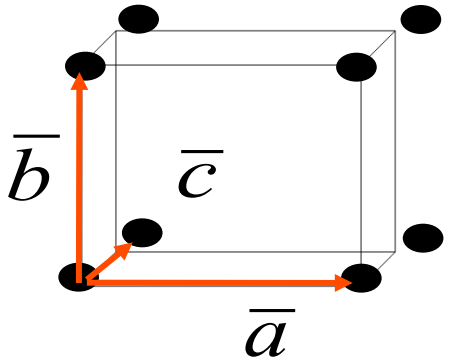
$$\vec{a}_3 = \frac{1}{2}(\hat{x} - \hat{y} + \hat{z})$$

Primitive and conventional cells



Body centered cubic (bcc):
conventional ≠primitive cell

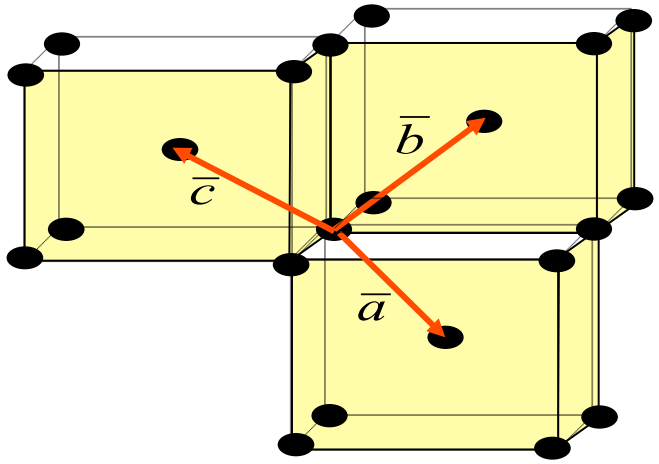
Fractional coordinates of lattice points in conventional cell:
000,100, 010, 001, 110,101, 011, 111, ½ ½ ½



Simple cubic (sc):
primitive cell=conventional cell

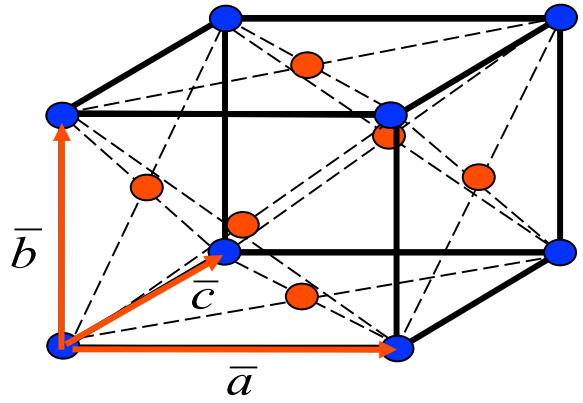
Fractional coordinates of lattice points:
000, 100, 010, 001, 110,101, 011, 111

Primitive and conventional cells



Body centered cubic (bcc):
primitive (rombohedron) ≠conventional cell

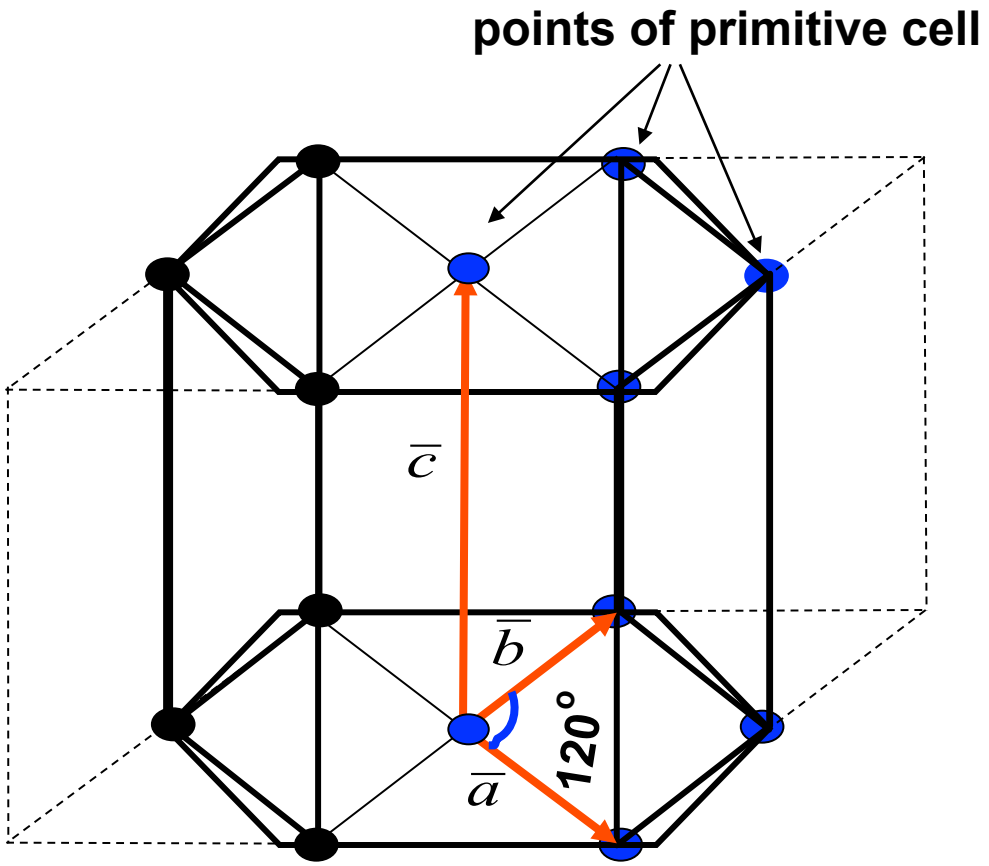
Fractional coordinates:
000, 100, 101, 110, 110,101, $0\bar{1}1$, $21\bar{1}$, $20\bar{0}$



Face centered cubic (fcc):
conventional ≠ primitive cell

Fractional coordinates:
000,100, 010, 001, 110,101, 011,111, ½ ½ 0, ½ 0 ½, 0 ½ ½ ,½1 ½ , 1 ½ ½ , ½ ½ 1

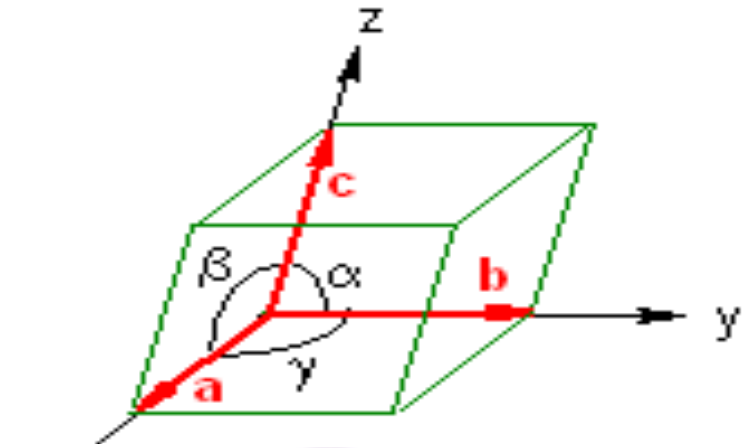
Primitive and conventional cells-hcp



Hexagonal close packed cell (hcp):
conventional =primitive cell

Fractional coordinates:
100, 010, 110, 101,011, 111,000, 001

Unit Cell



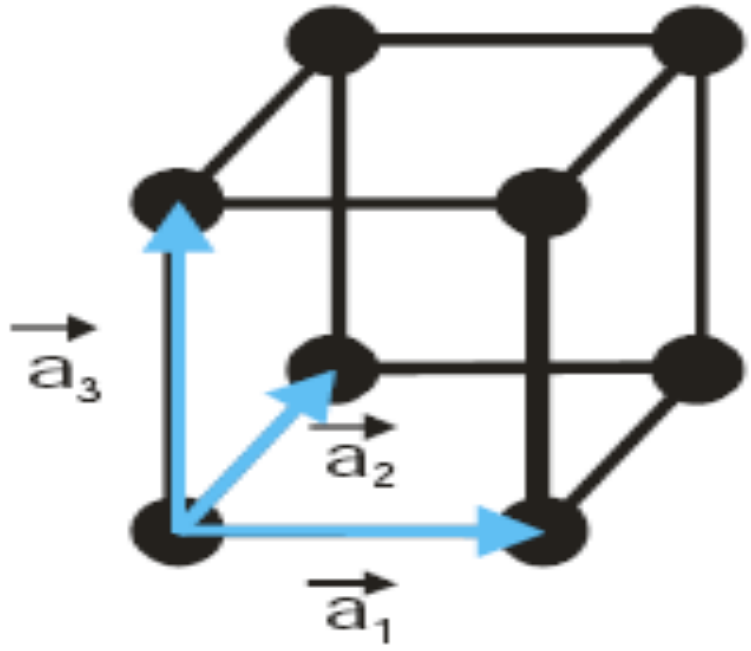
- The unit cell and, consequently, the entire lattice, is *uniquely* determined by the six lattice constants: a, b, c, α, β and γ.
- Only 1/8 of each lattice point in a unit cell can actually be assigned to that cell.
- Each unit cell in the figure can be associated with 8 x 1/8 = 1 lattice point.

Primitive Unit Cell and vectors

- A primitive unit cell is made of primitive translation vectors a_1 ,a_2, and a_3 such that there is no cell of smaller volume that can be used as a building block for crystal structures.

- A primitive unit cell will fill space by repetition of suitable crystal translation vectors. This defined by the parallelpiped a_1, a_2 and a_3. The volume of a primitive unit cell can be found by

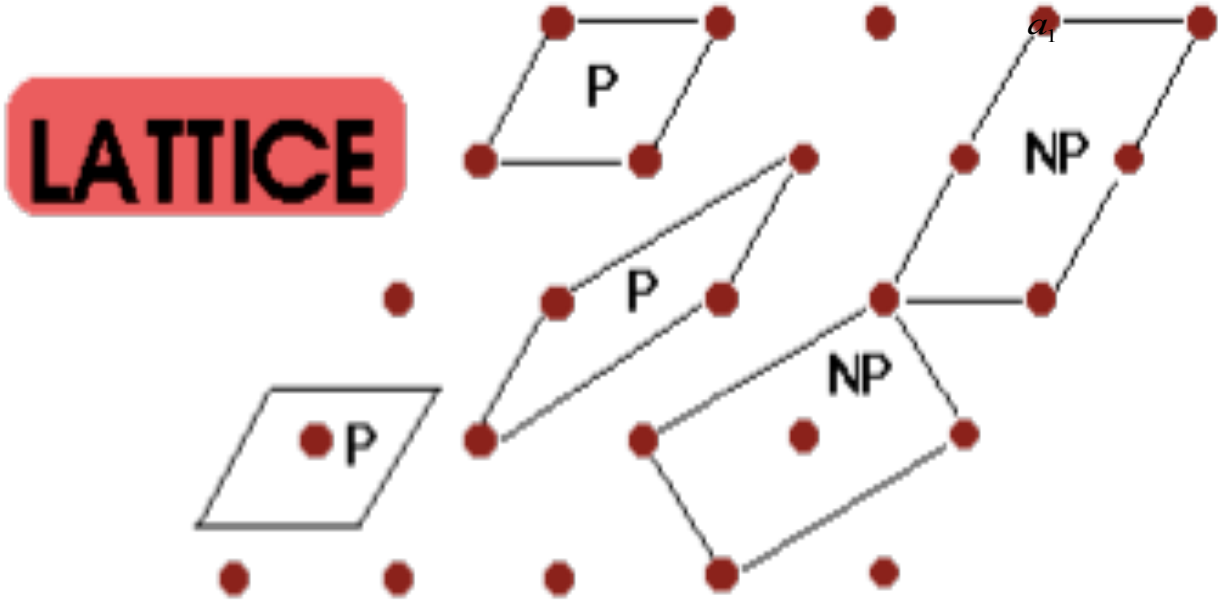
- $V = a_1.(a_2 \times a_3)$ (vector products)



Cubic cell volume = a^3

Primitive Unit Cell

- The primitive unit cell must have only one lattice point.
- There can be different choices for lattice vectors , but the volumes of these primitive cells are all the same.



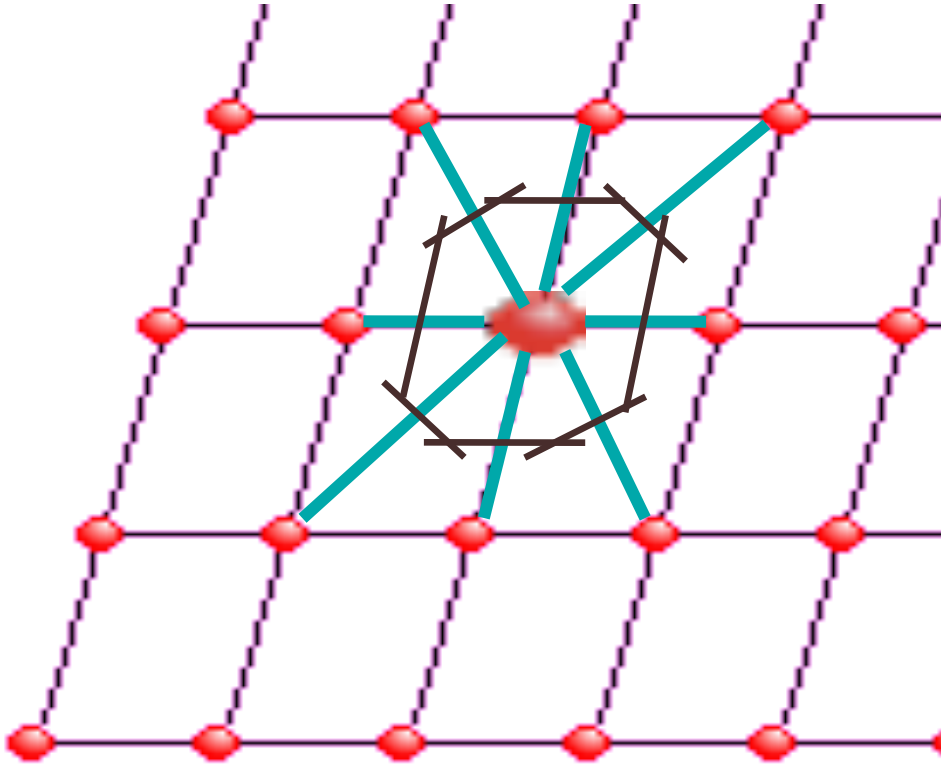
P = Primitive Unit Cell
NP = Non-Primitive Unit Cell

Wigner-Seitz Method

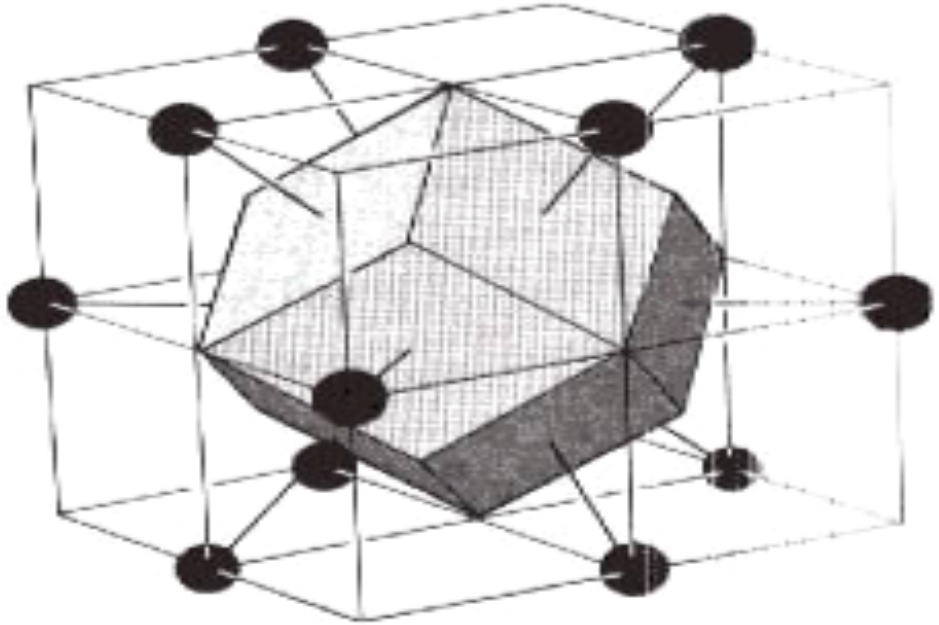
A simply way to find the primitive cell which is called Wigner-Seitz cell can be done as follows;

1. **Choose a lattice point.**
2. **Draw lines to connect these lattice point to its neighbours.**
3. **At the mid-point and normal to these lines draw new lines.**

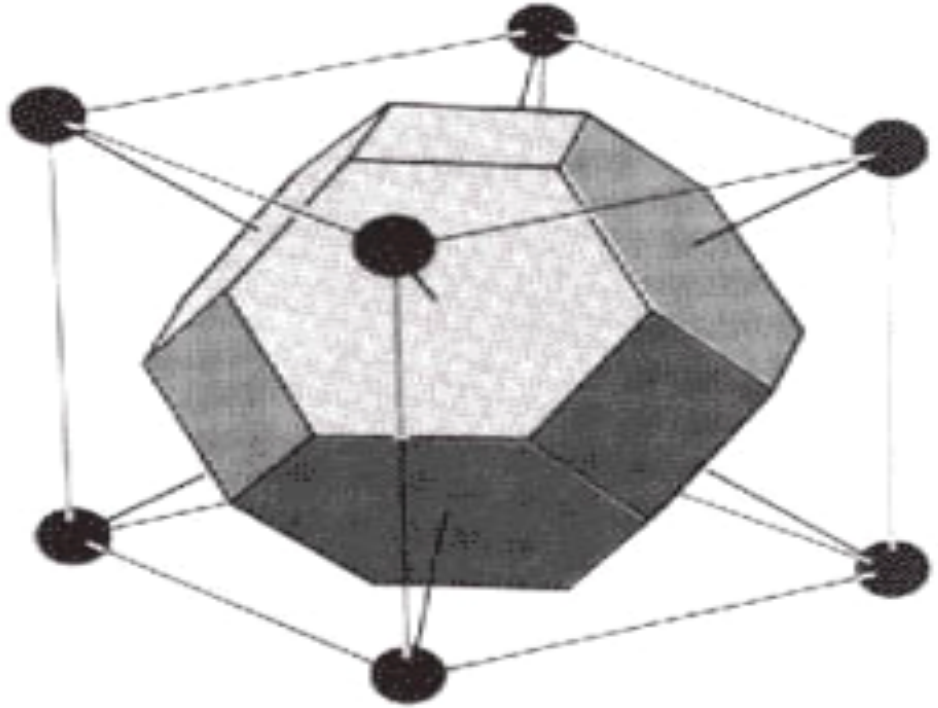
The volume enclosed is called as a Wigner-Seitz cell.



Wigner-Seitz Cell - 3D

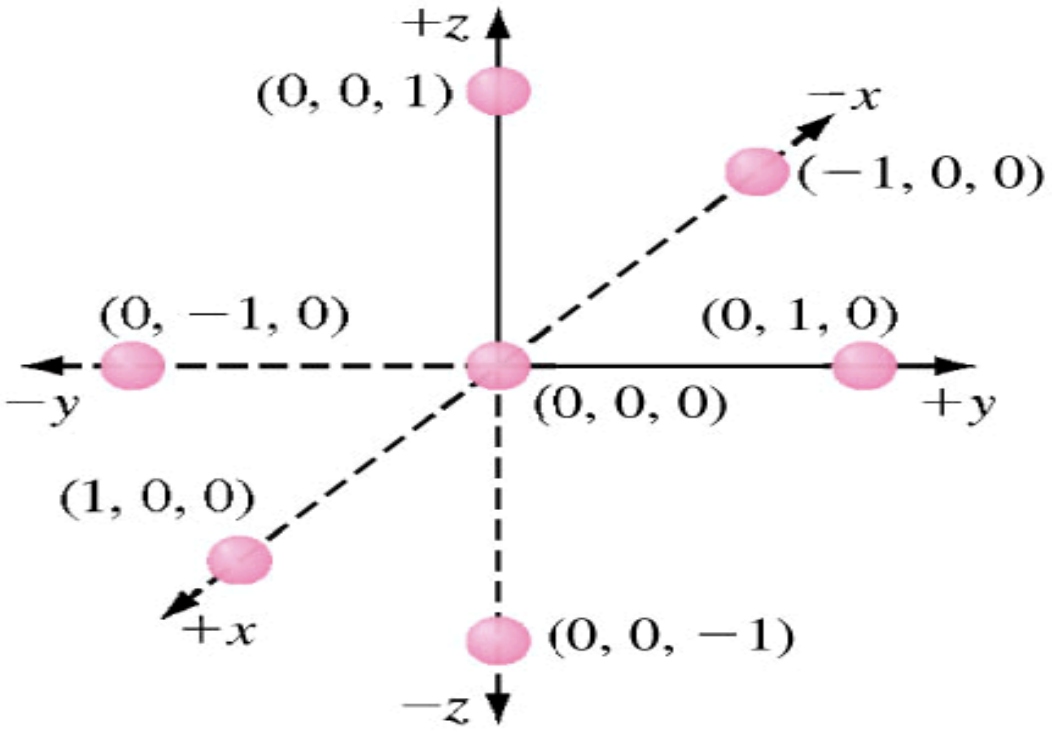


f.c.c Wigner-Seitz cell

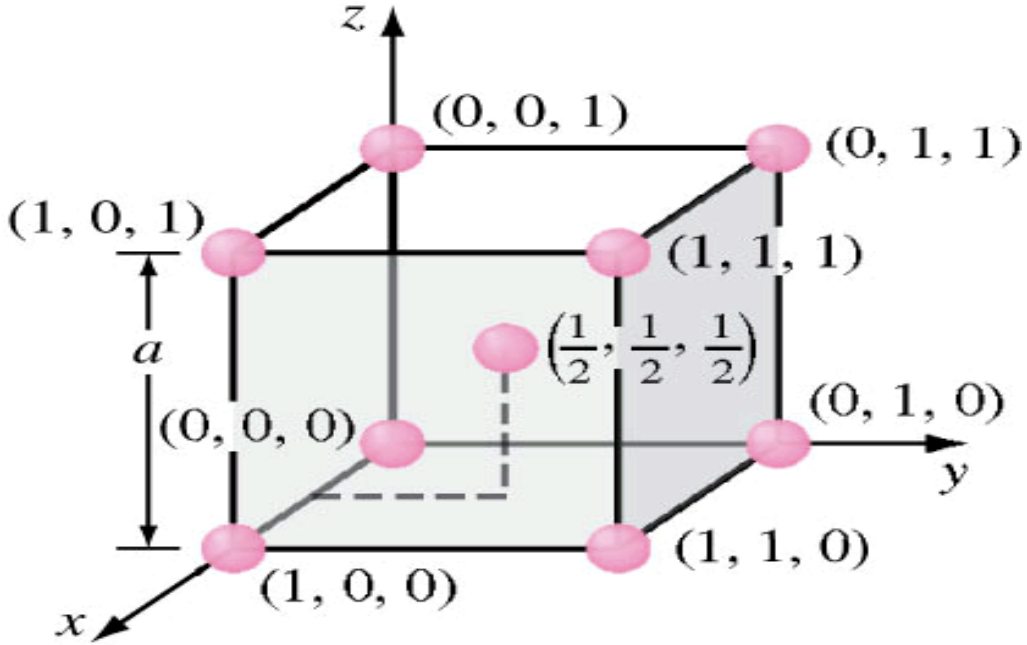


b.c.c Wigner-Seitz cell

Lattice Sites in Cubic Unit Cell



(a)



(b)

Crystal Directions

- We choose one lattice point on the line as an origin, say the point O. Choice of origin is completely arbitrary, since every lattice point is identical.
- Then we choose the lattice vector joining O to any point on the line, say point T. This vector can be written as;

$$R = n_1 a + n_2 b + n_3 c$$

- To distinguish a lattice direction from a lattice point, the triple is enclosed in square brackets [...] is used.$[n_1 n_2 n_3]$
- $[n_1 n_2 n_3]$ is the smallest integer of the *same relative ratios*.

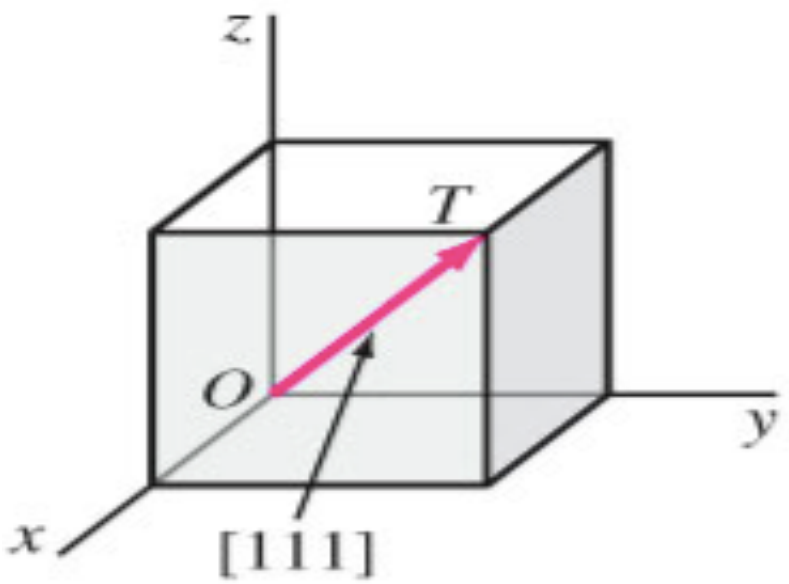


Fig. Shows [111] direction