STRUKTUR KRISTAL

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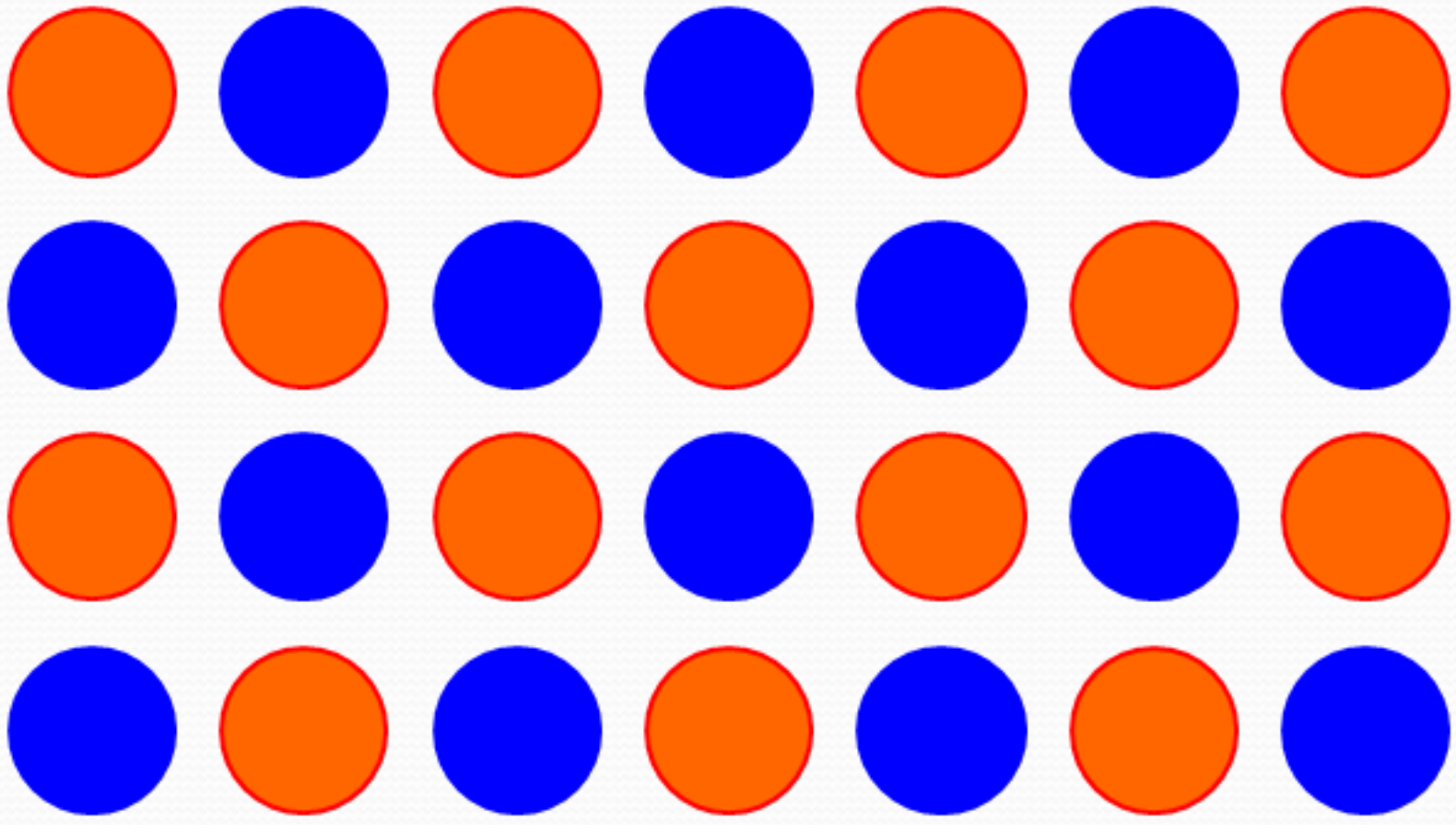
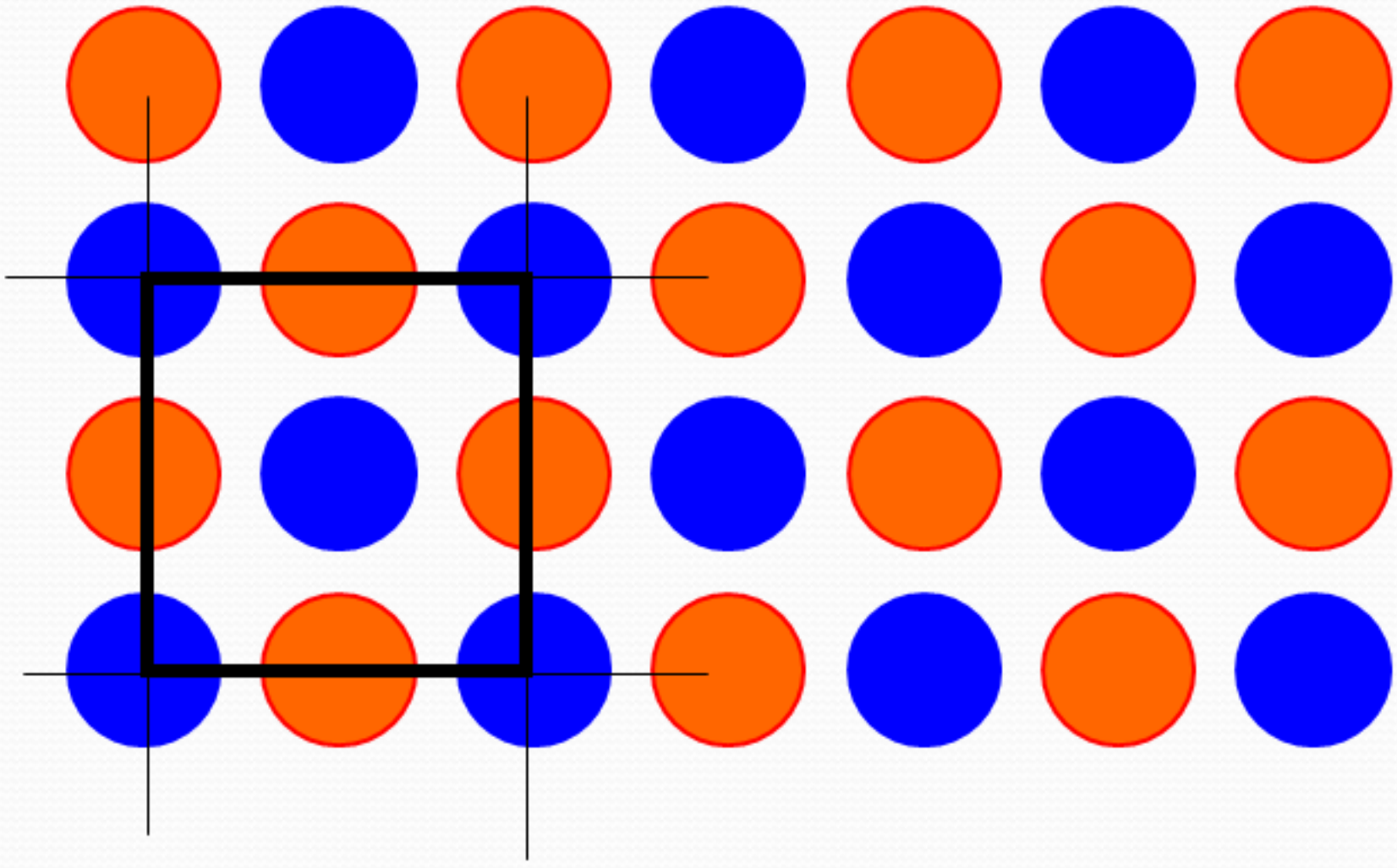
2012

2D Unit Cell example -(NaCl)

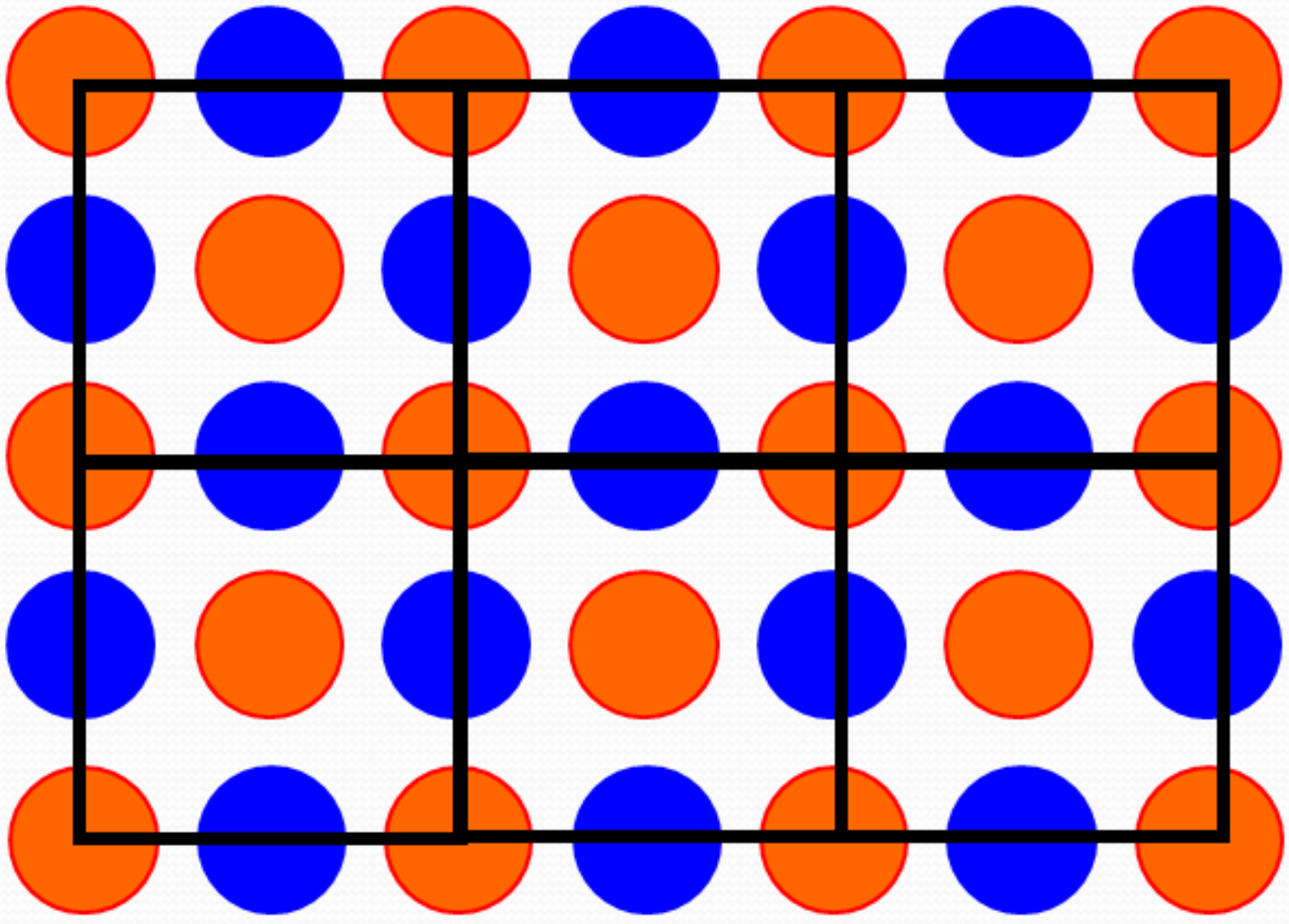


We define lattice points ; these are points with *identical environments*

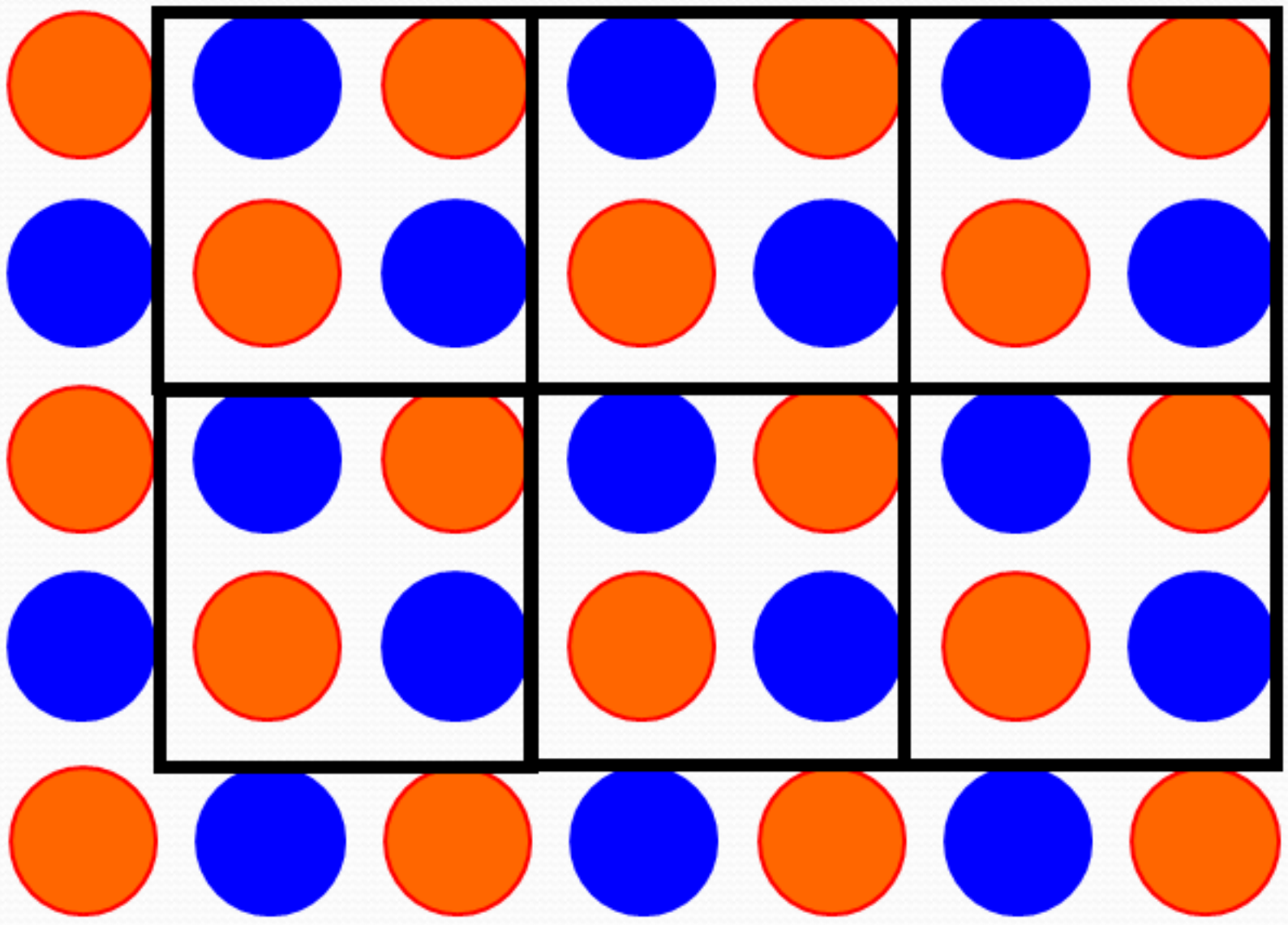
Choice of origin is arbitrary - lattice points need not be atoms - **but** unit cell size should always be the same.



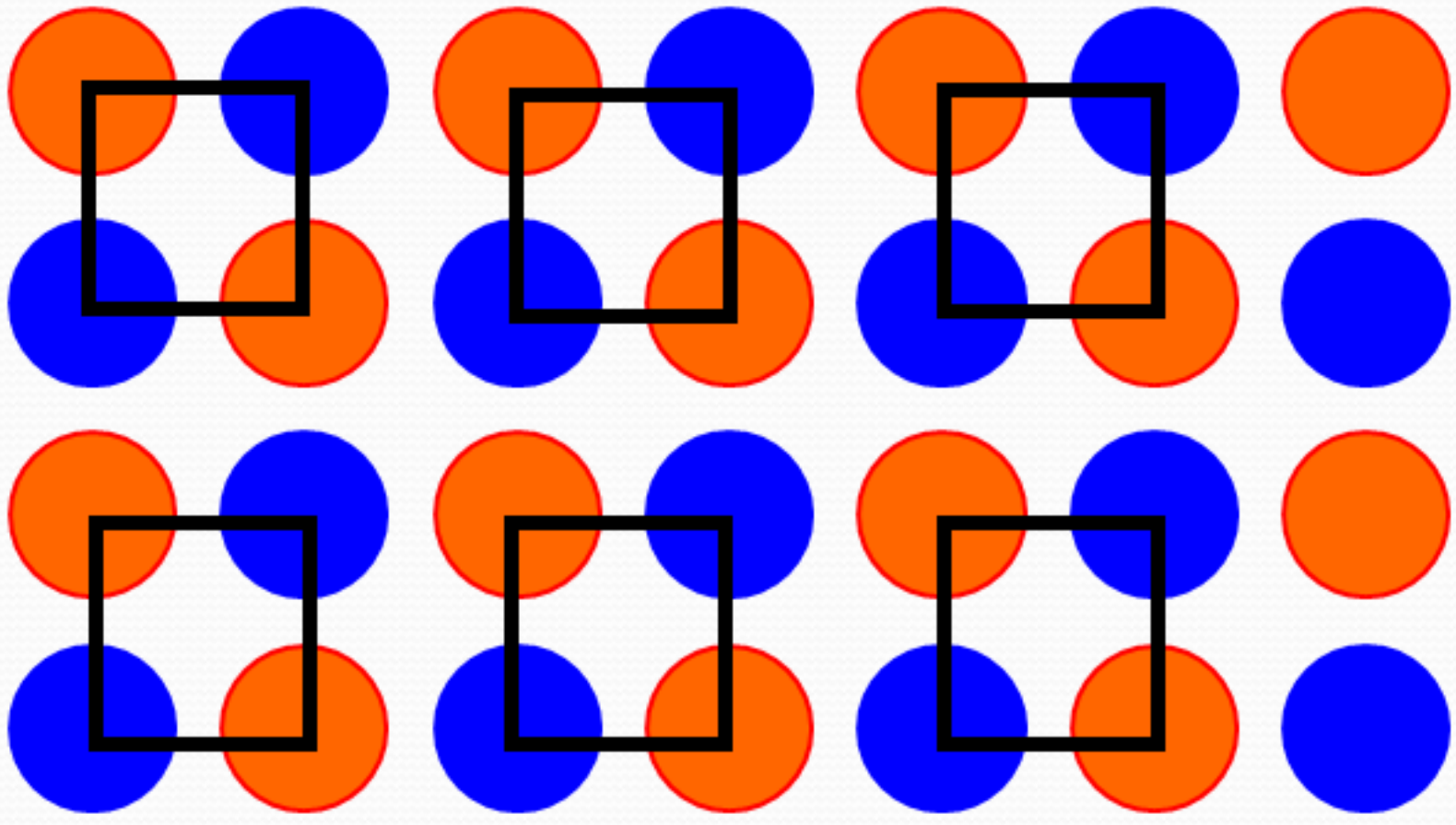
This is also a unit cell -
it doesn't matter if you start from Na or Cl



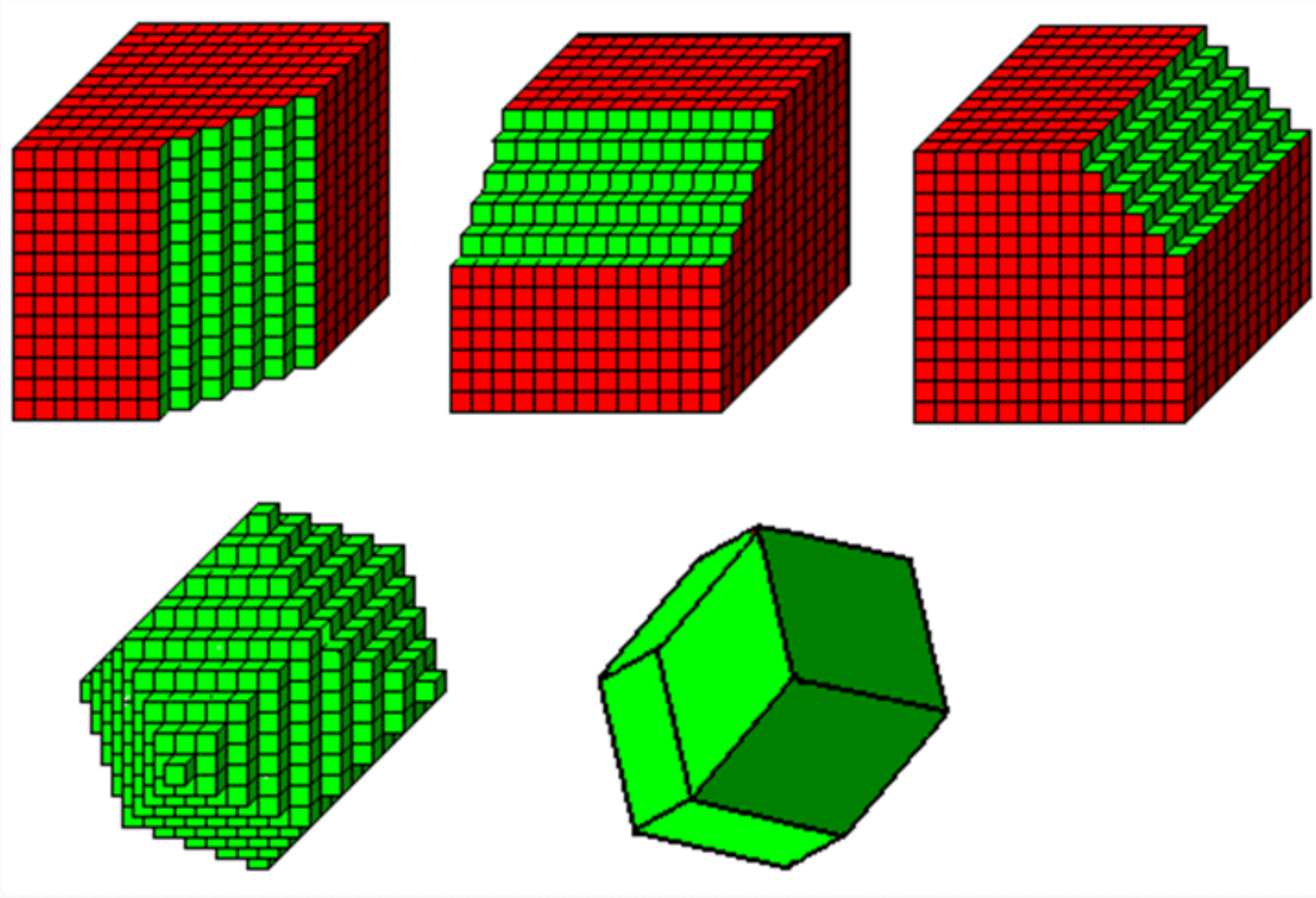
- or if you don't start from an atom



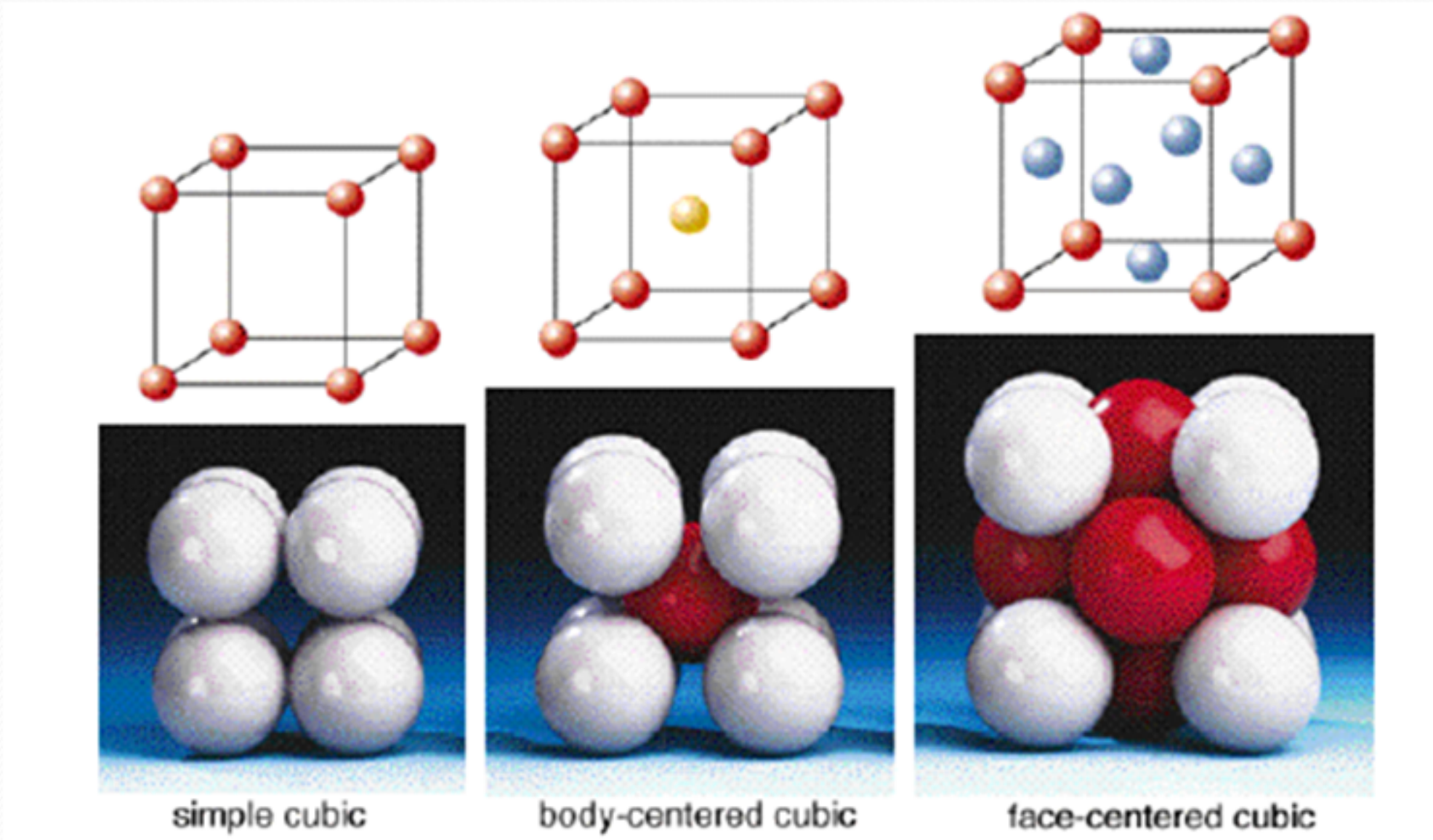
This is NOT a unit cell even though they are all the same - empty space is not allowed!



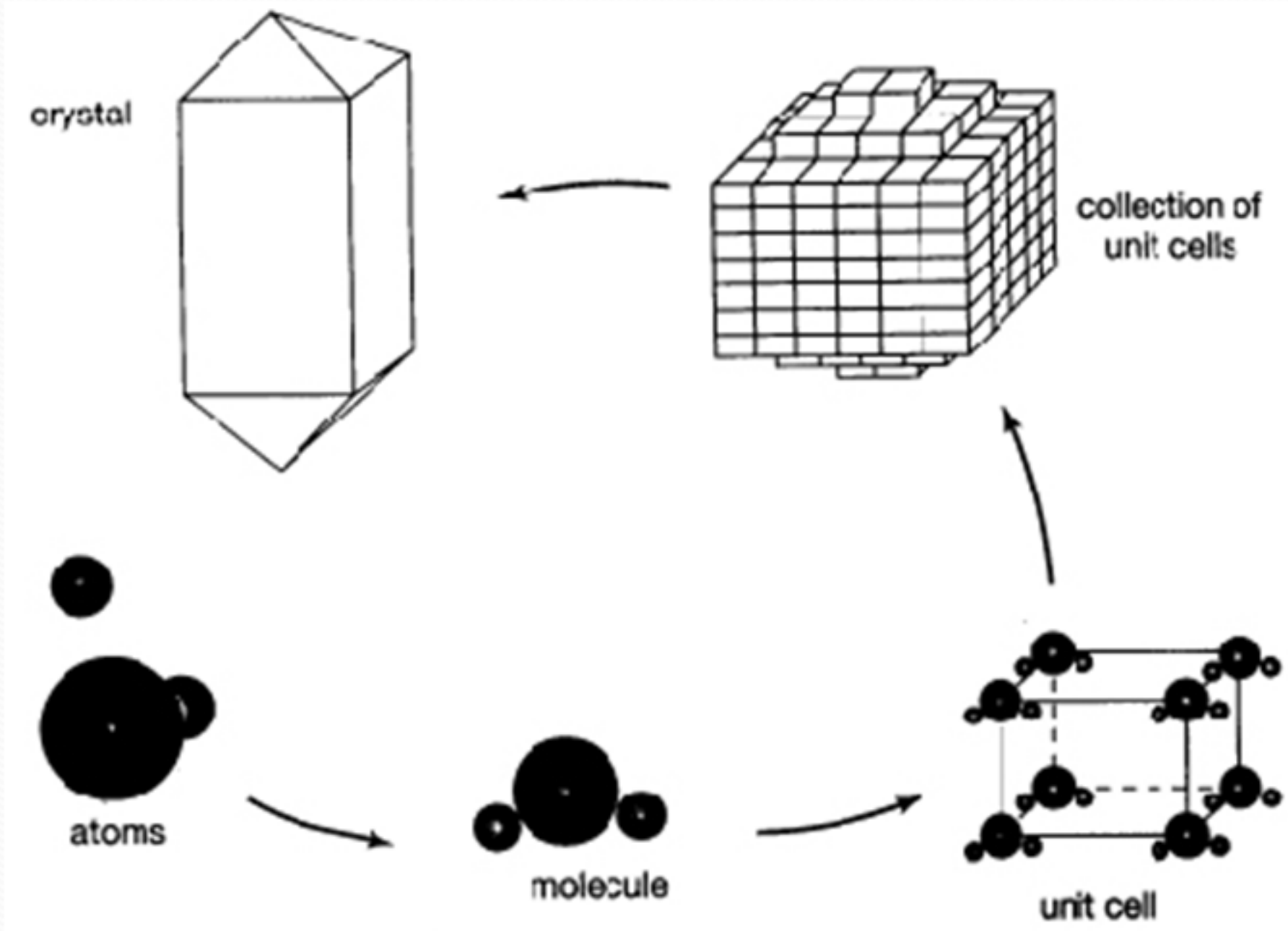
Unit Cell in 3D



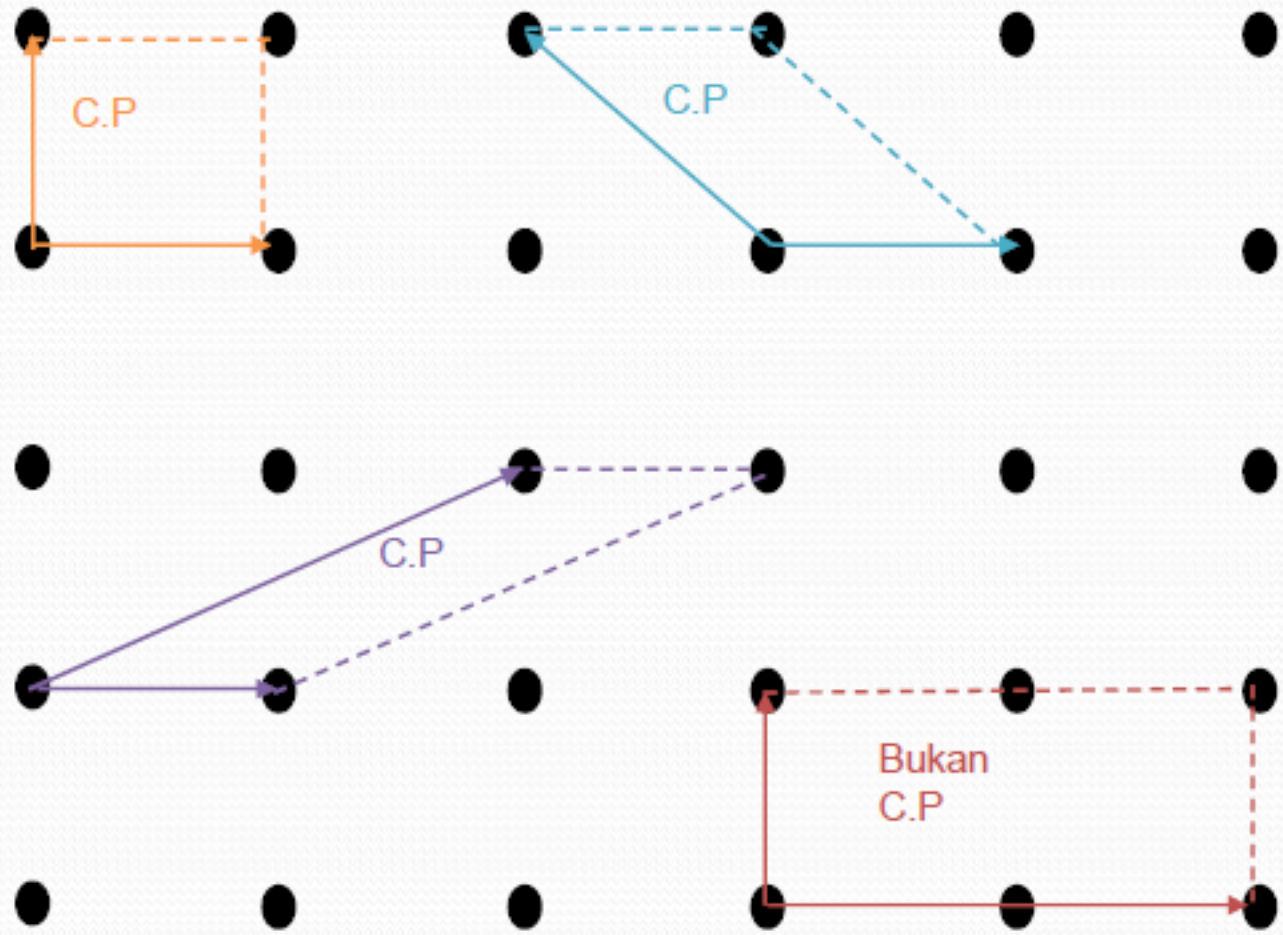
Three common Unit Cells in 3D



Unit Cell in 3D



Cara menentukan sel primitif



Primitive Unit Cell

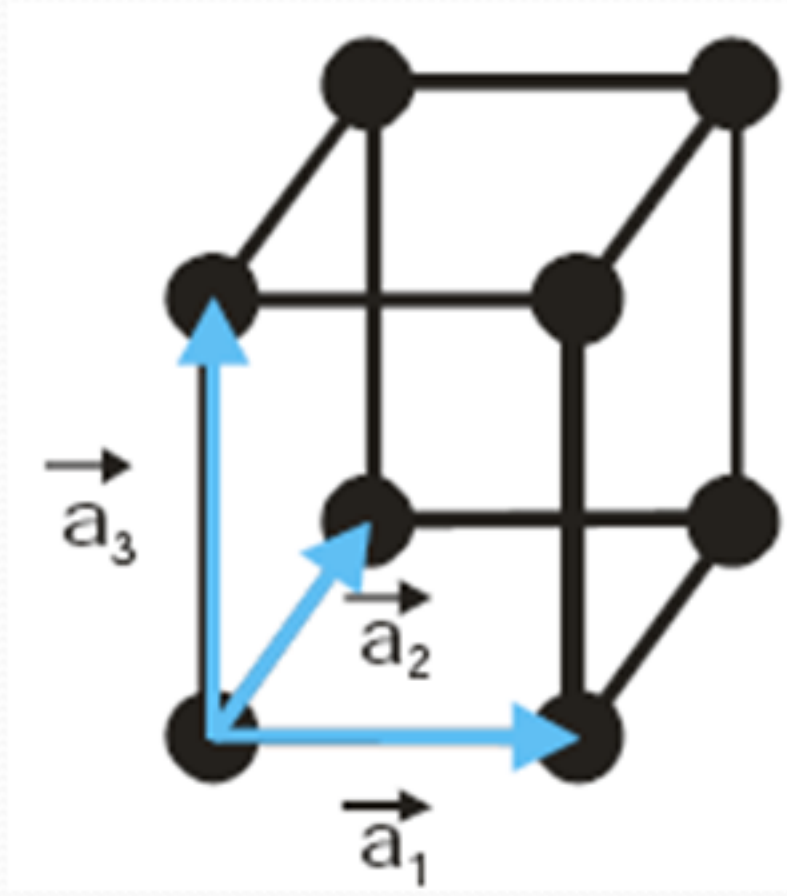
- A **primitive cell** or **primitive unit cell** is a volume of space that when translated through all the vectors in a Bravais lattice just fills all of space without either overlapping itself or leaving voids.
- A primitive cell must contain precisely one lattice point.

- Solids consist of atoms or molecules ***executing thermal motion*** about an equilibrium position ***fixed at a point*** in space.

- Solids can take the form of crystalline, polycrstalline, or amorphous materials.
- Solids (at a given temperature, pressure, and volume) have stronger bonds between molecules and atoms than liquids.
- Solids require more energy to ***break the bonds.***

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.



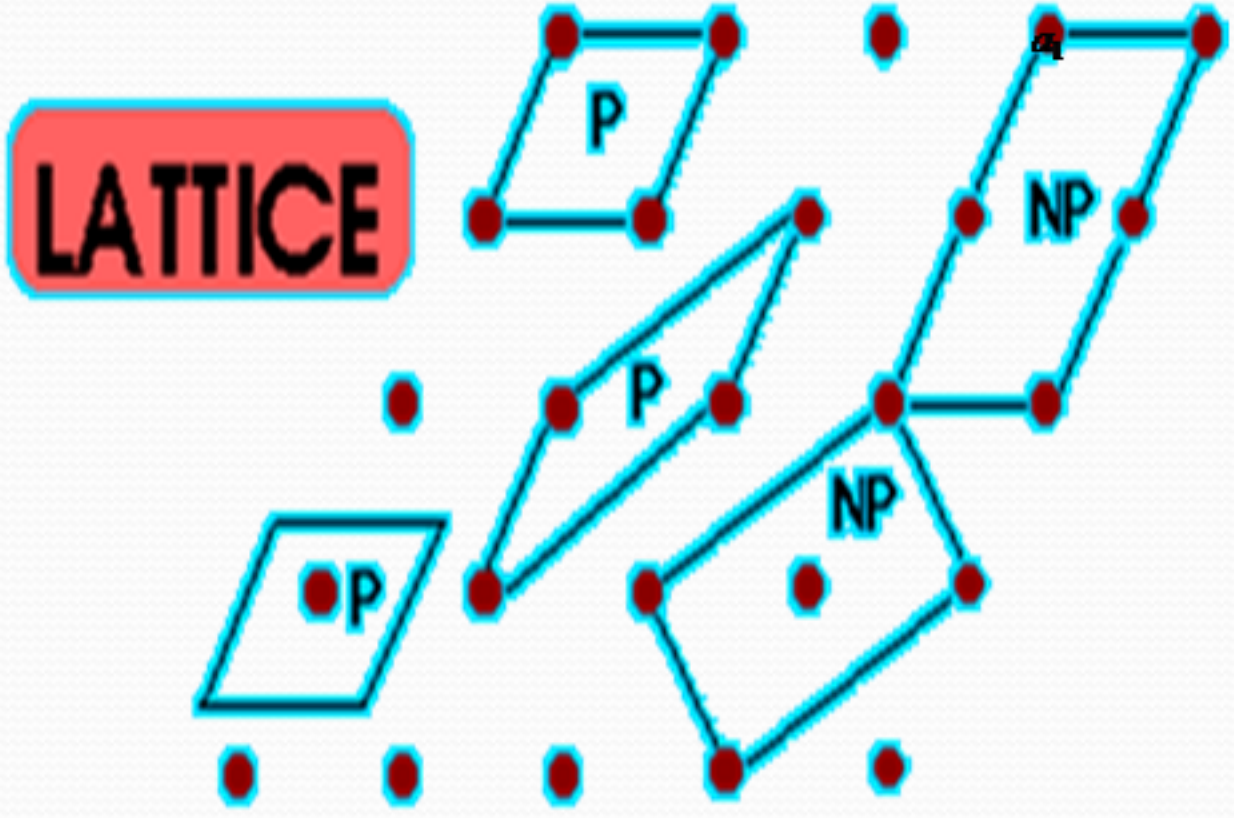
- **A primitive unit cell will fill space by repetition of suitable crystal translation vectors. This defined by the parallelpiped a_1, a_2 and a_3. The volume of a primitive unit cell can be found by**

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

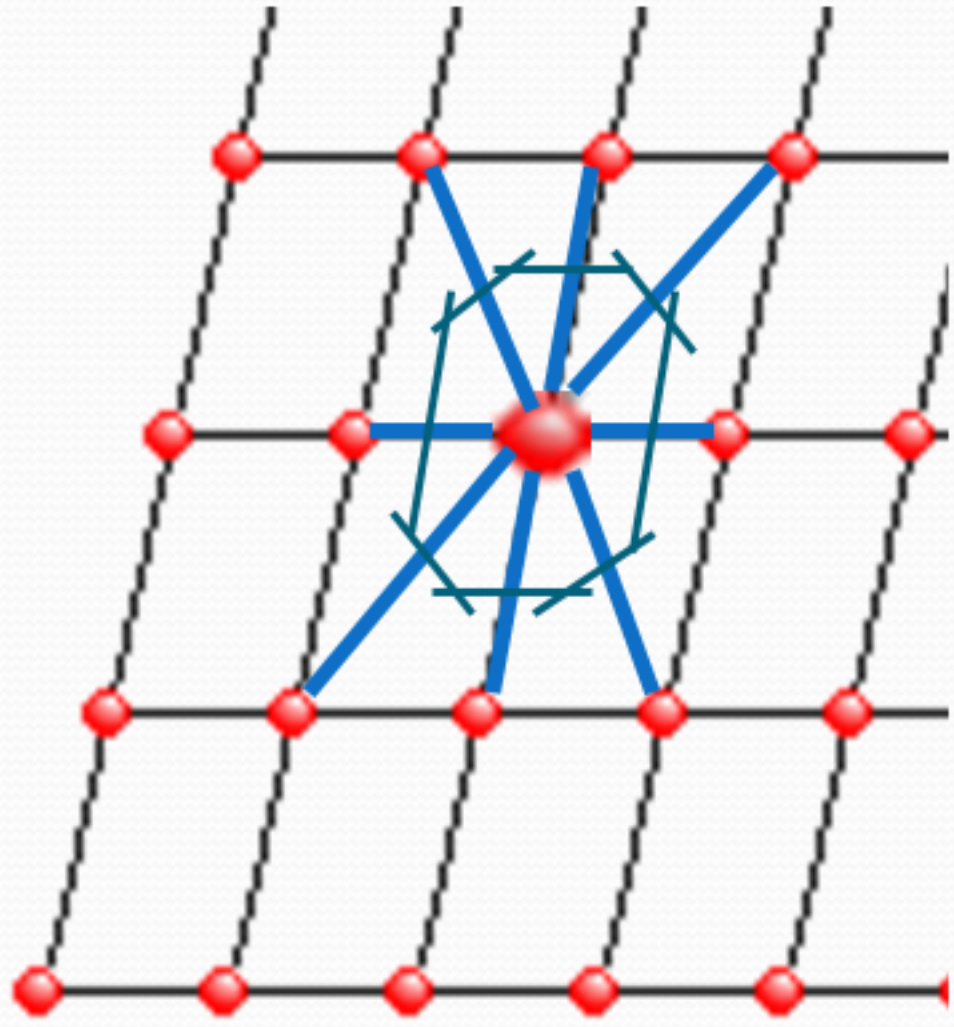


P = Primitive Unit Cell
NP = Non-Primitive Unit Cell

Wigner-Seitz Method

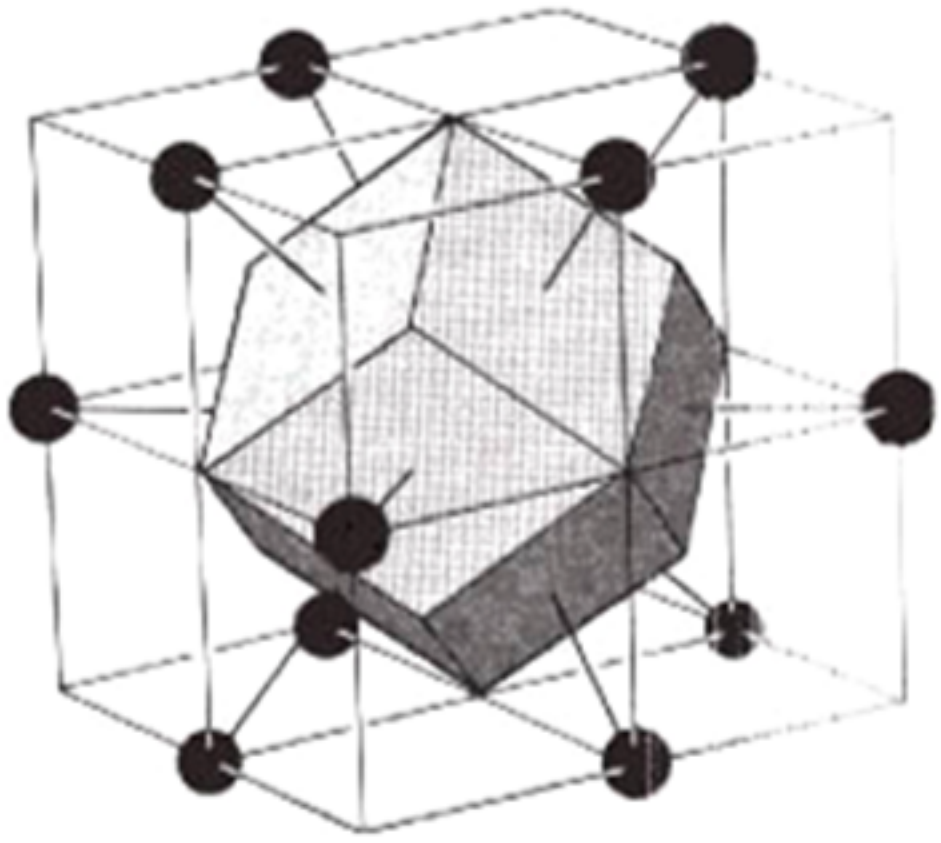
A simply way to find the primitive cell which is called Wigner-Seitz cell can be done as follows;

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.

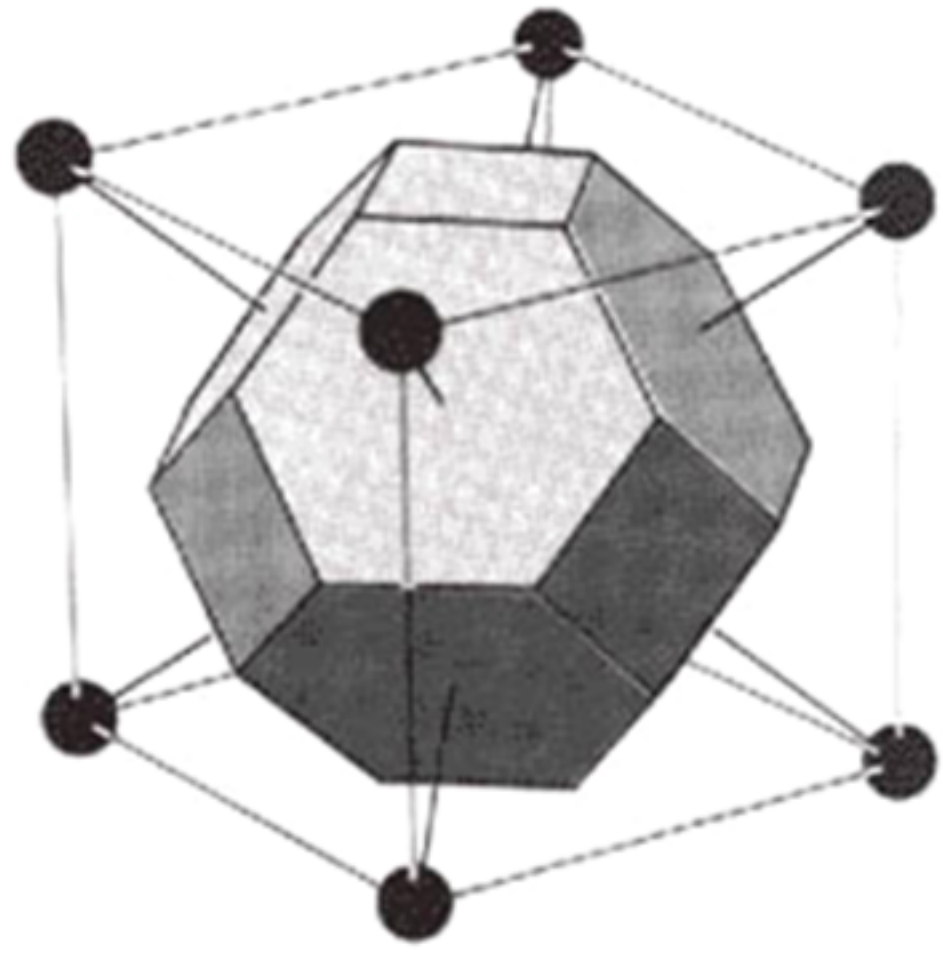


The volume enclosed is called as a Wigner-Seitz cell.

Wigner-Seitz Cell - 3D



f.c.c Wigner-Seitz cell



b.c.c Wigner-Seitz cell

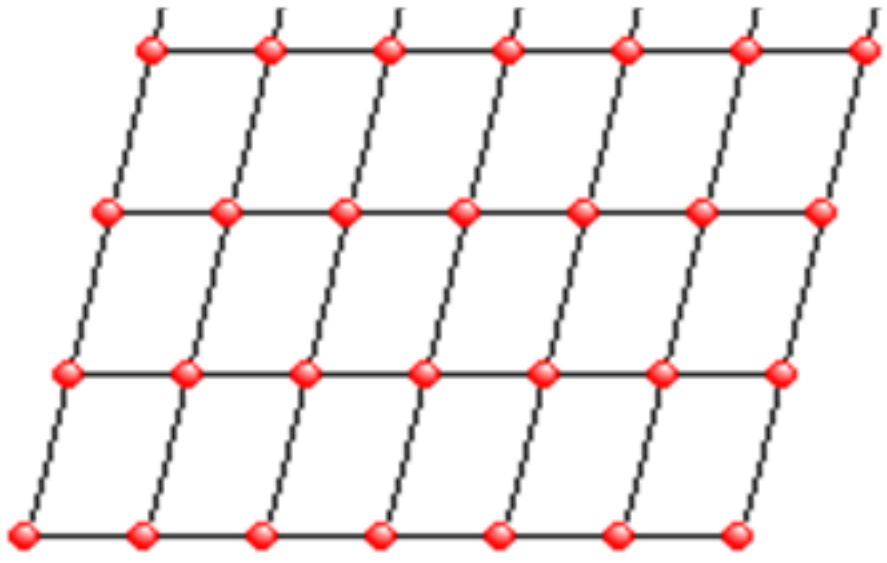
Fundamental Types of Lattices

- Crystal lattices can be mapped into themselves by the lattice translations **T** and by various other symmetry operations.
- A typical symmetry operation is that of rotation about an axis that passes through a lattice point. Allowed rotations of : 2 π, 2π/2, 2π/3,2π/4, 2π/6
- (Note: lattices do not have rotation axes for 1/5, 1/7 ...) times 2π

Crystal Lattice

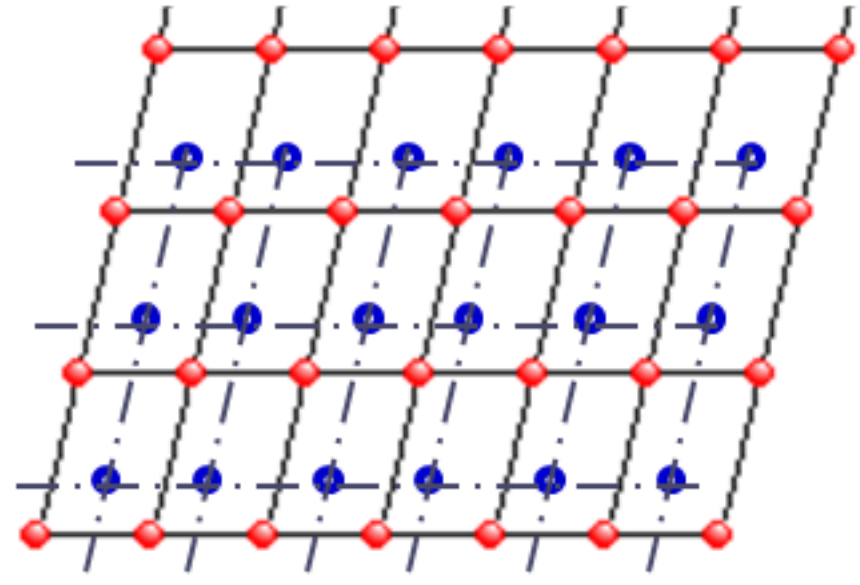
Bravais Lattice (BL)

§ All atoms are of the same kind
§ All lattice points are equivalent



Non-Bravais Lattice (non-BL)

§ Atoms can be of different kind
§ Some lattice points are not equivalent
§A combination of two or more BL



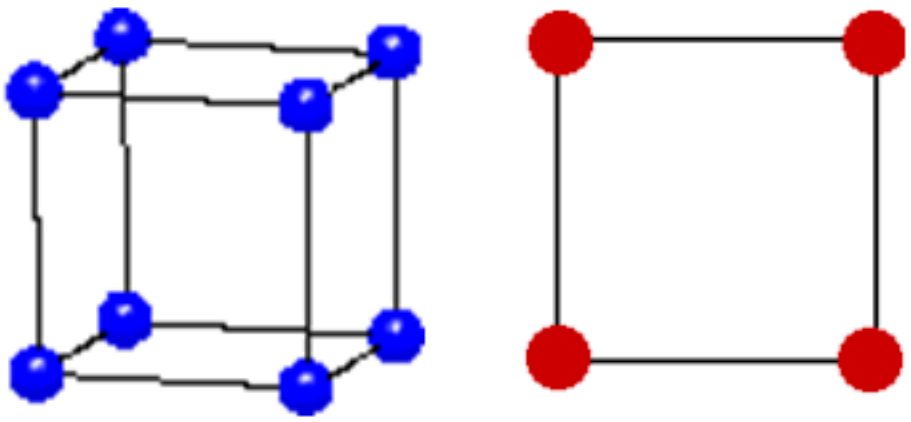
UNIT CELL

Primitive

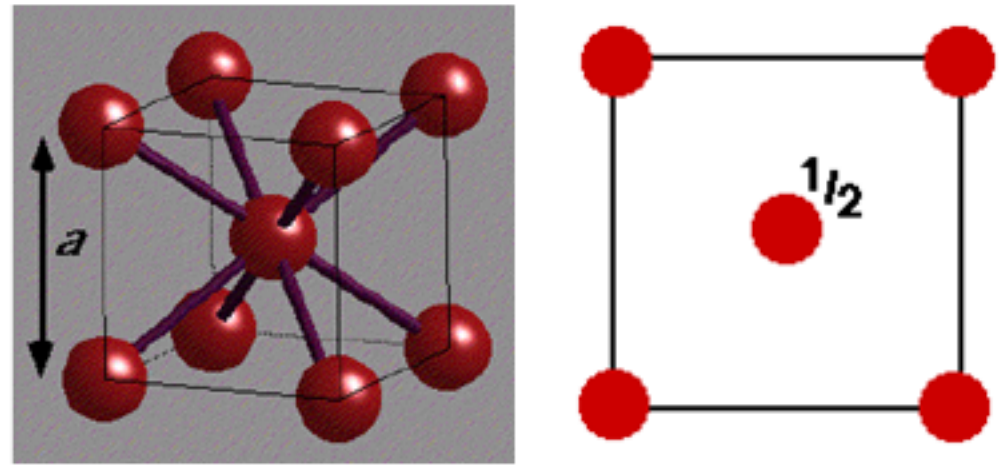
§ Single lattice point per cell
§ Smallest area in 2D, or
§Smallest volume in 3D

Conventional & Non-primitive

§ More than one lattice point per cell
§ Integral multibles of the area of primitive cell

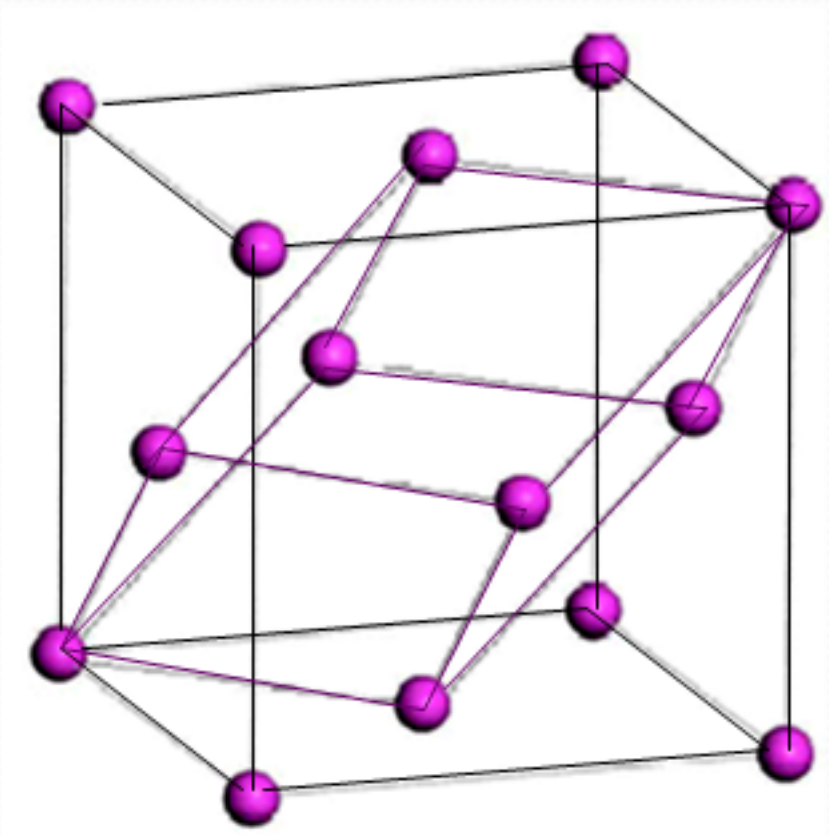


Simple cubic(sc)



Body centered cubic(bcc)

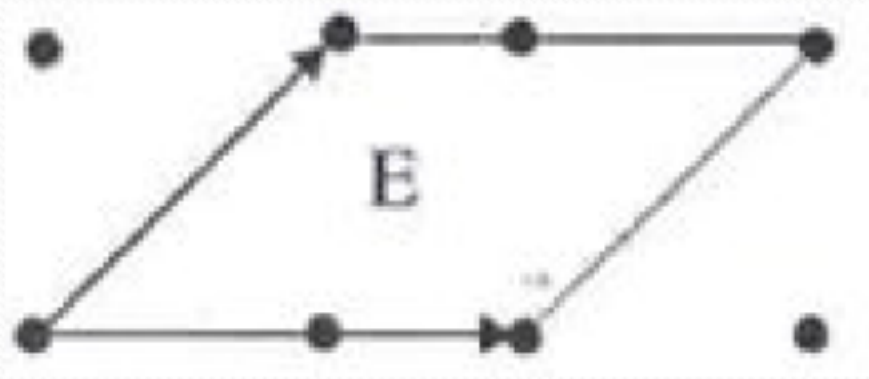
The Conventional Unit Cell



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.

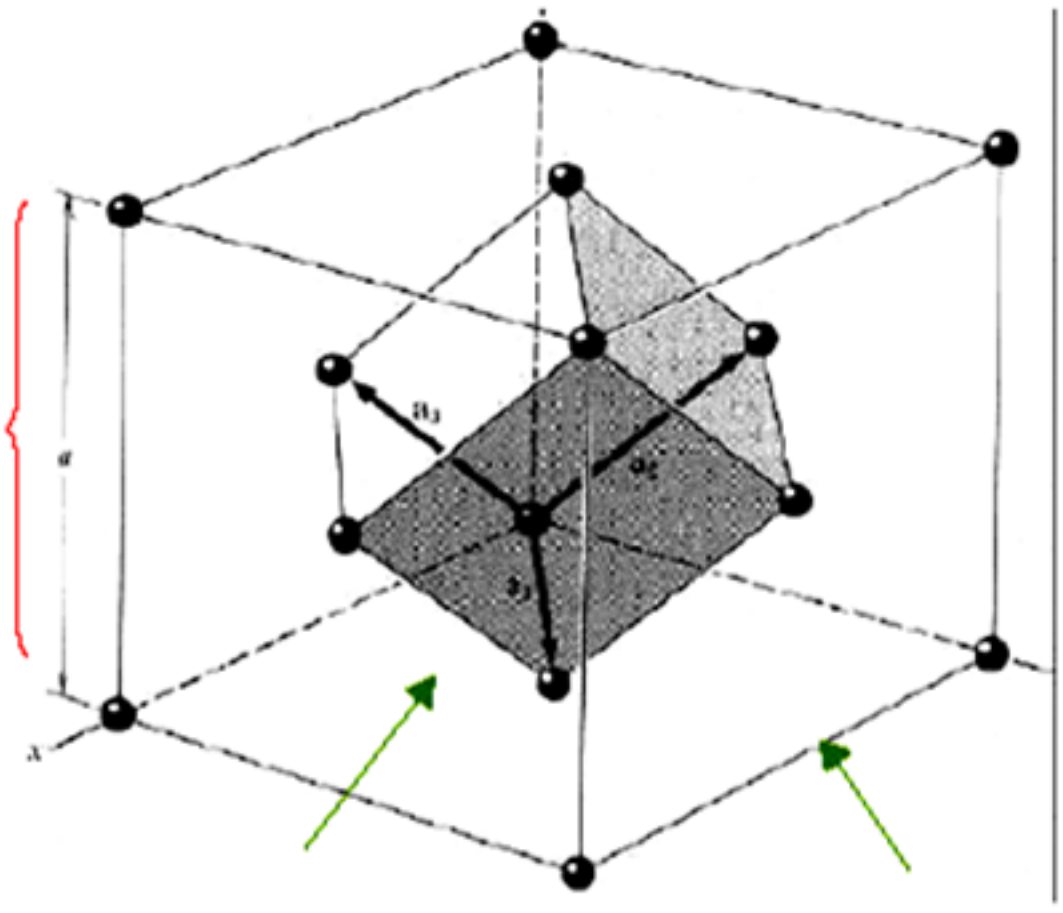
- sel konvensional (sel tak primitif) adalah sel yang mempunyai luas atau volume bukan terkecil artinya mempunyai luas atau volume yang besarnya merupakan kelipatan sel primitif.



Gambar sel konvensional

Primitive and conventional cells of FCC

lattice constant



primitive vectors

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

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

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

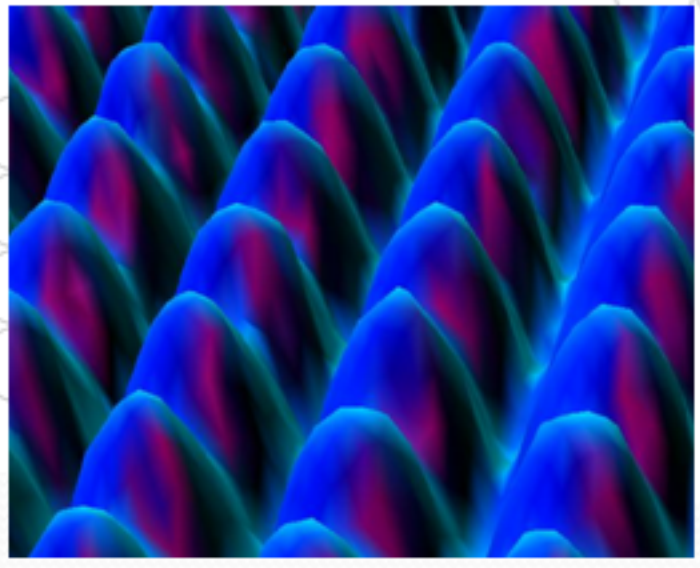
A primitive unit cell a conventional unit cell

CRYSTAL LATTICE

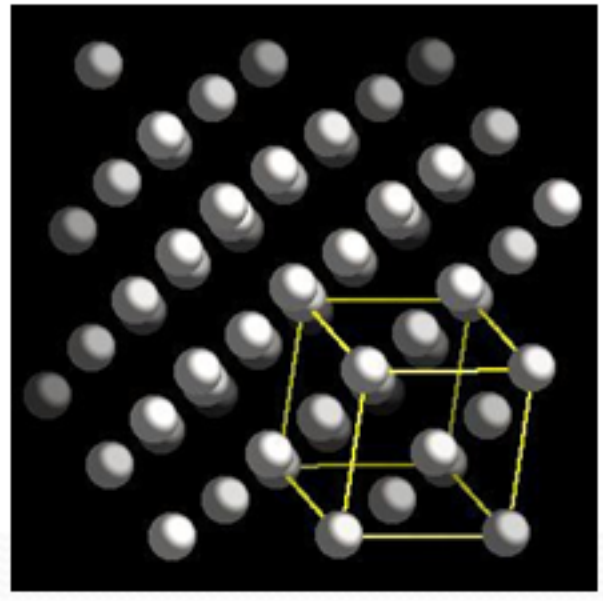
What is a crystal lattice?

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

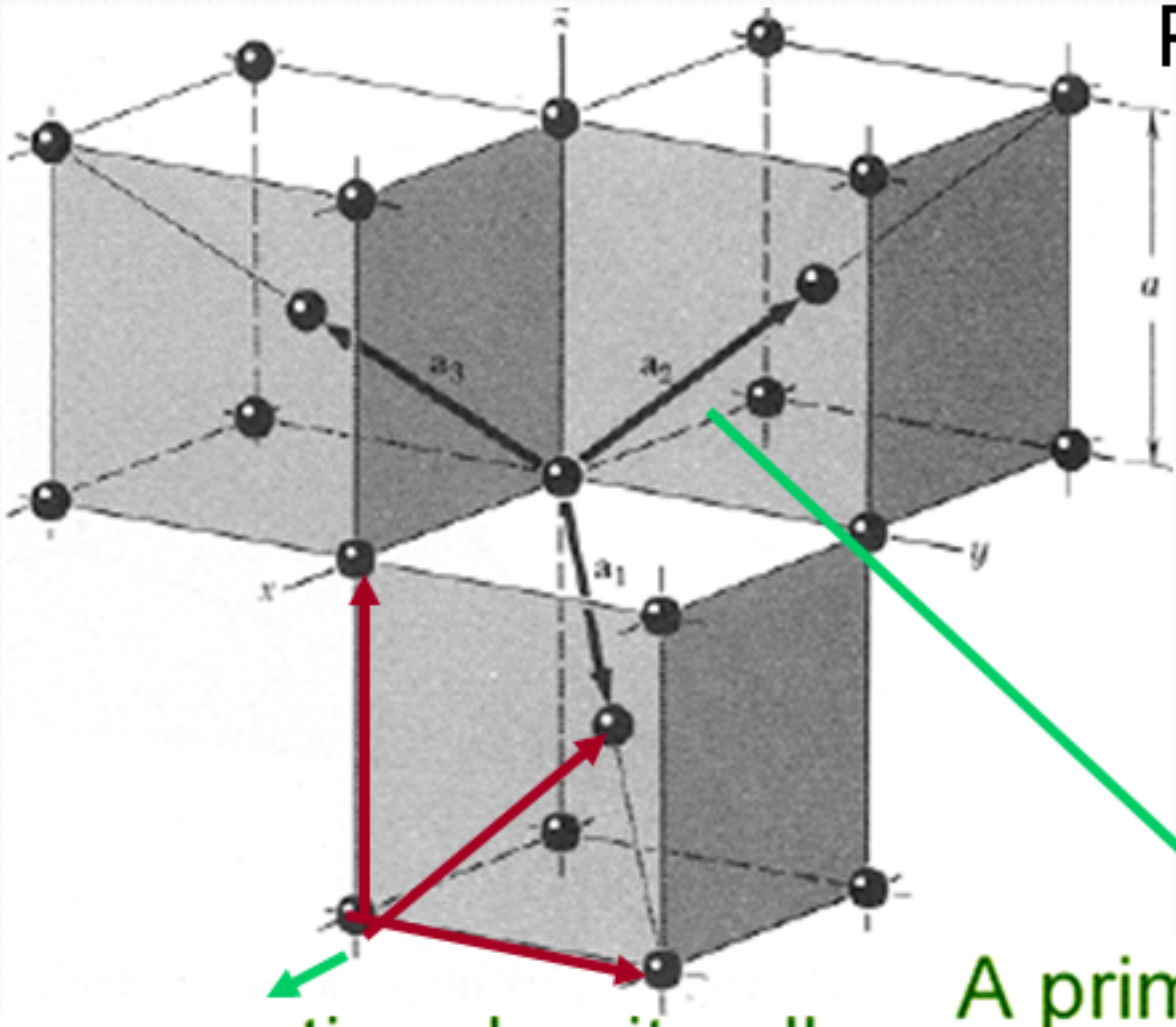


Platinum surface
(scanning tunneling microscope)



Crystal lattice and structure of Platinum

Primitive and conventional cells of BCC



a conventional unit cell

Primitive Translation Vectors:

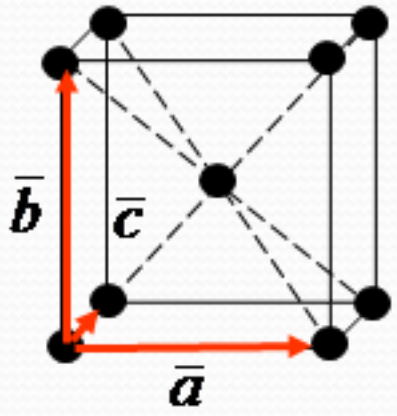
$$\vec{a}_1 = \frac{1}{2}(\hat{x} + \hat{y} - \hat{z})$$

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

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

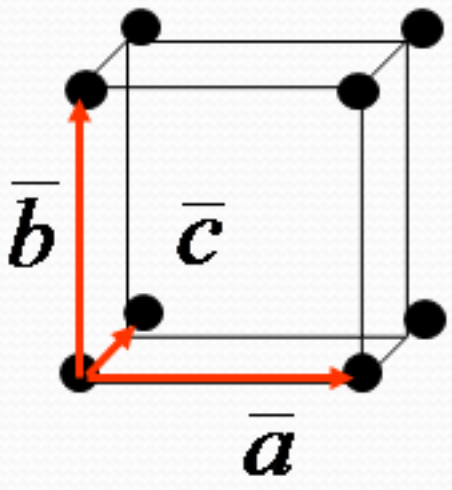
A primitive unit cell

Primitive and conventional cells



Body centered cubic (bcc):
conventional ≠primitive cell

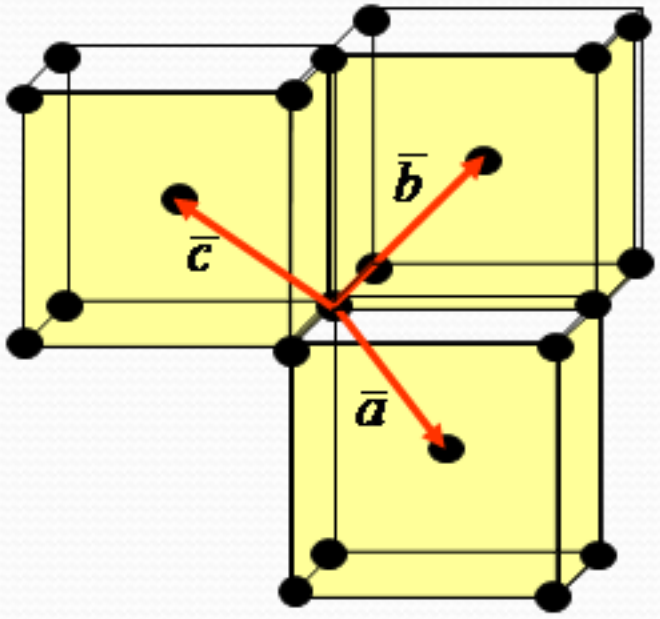
Fractional coordinates of lattice points in conventional cell:
000,100, 010, 001, 110,101, 011, 111, ½ ½ ½



Simple cubic (sc):
primitive cell=conventional cell

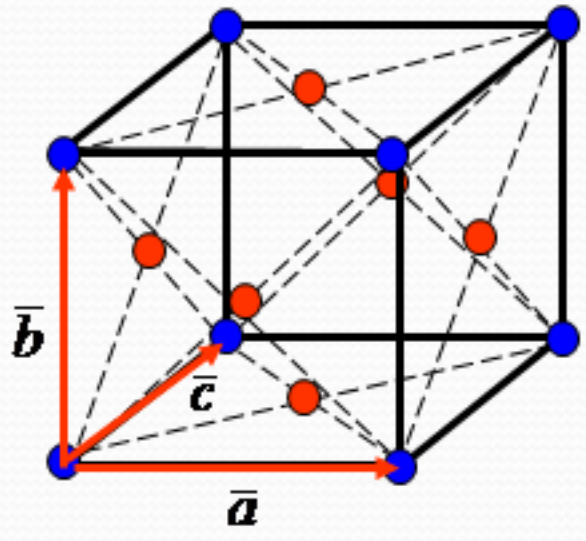
Fractional coordinates of lattice points:
000, 100, 010, 001, 110,101, 011, 111

Primitive and conventional cells



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

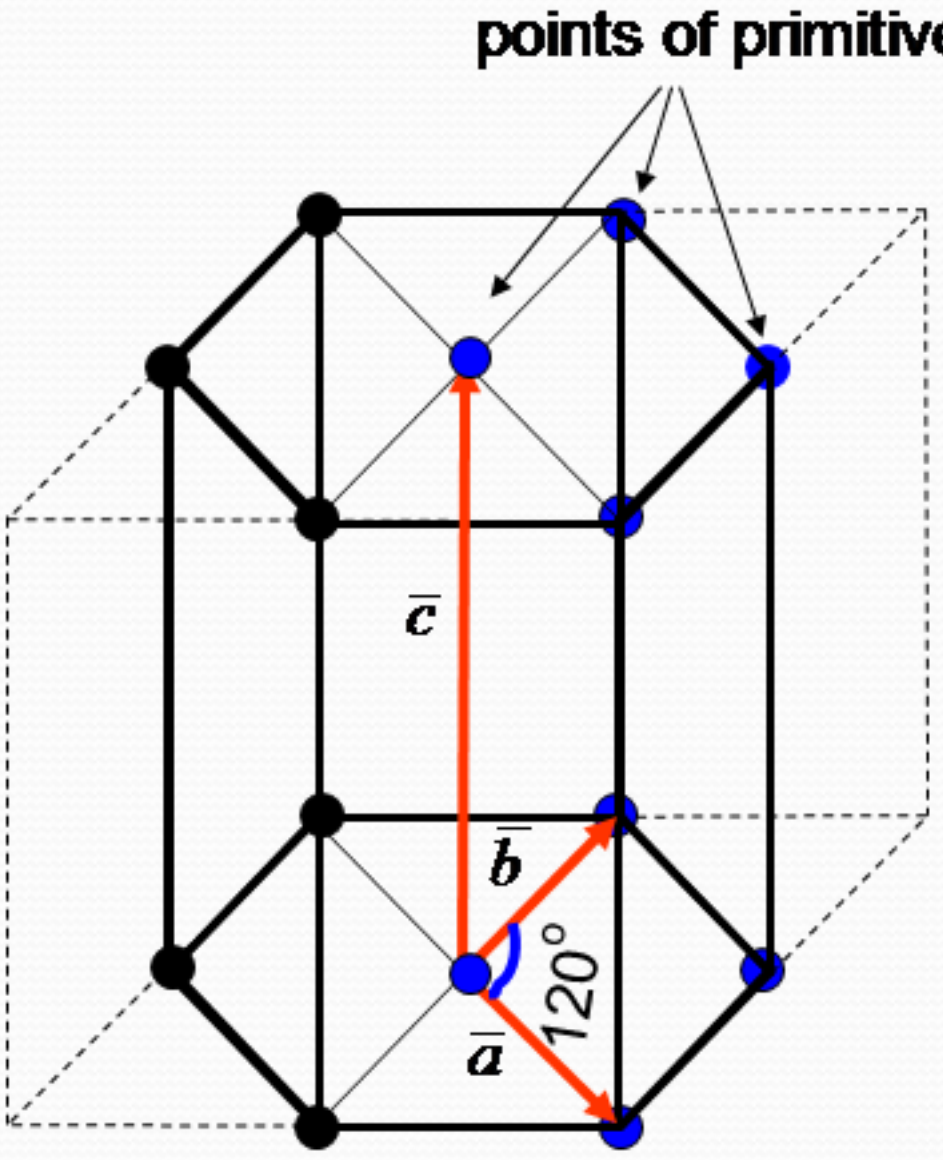
Fractional coordinates:
000, 100, 101, 110, $1\bar{1}0$, $10\bar{1}$, $01\bar{1}$, 211, 200



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

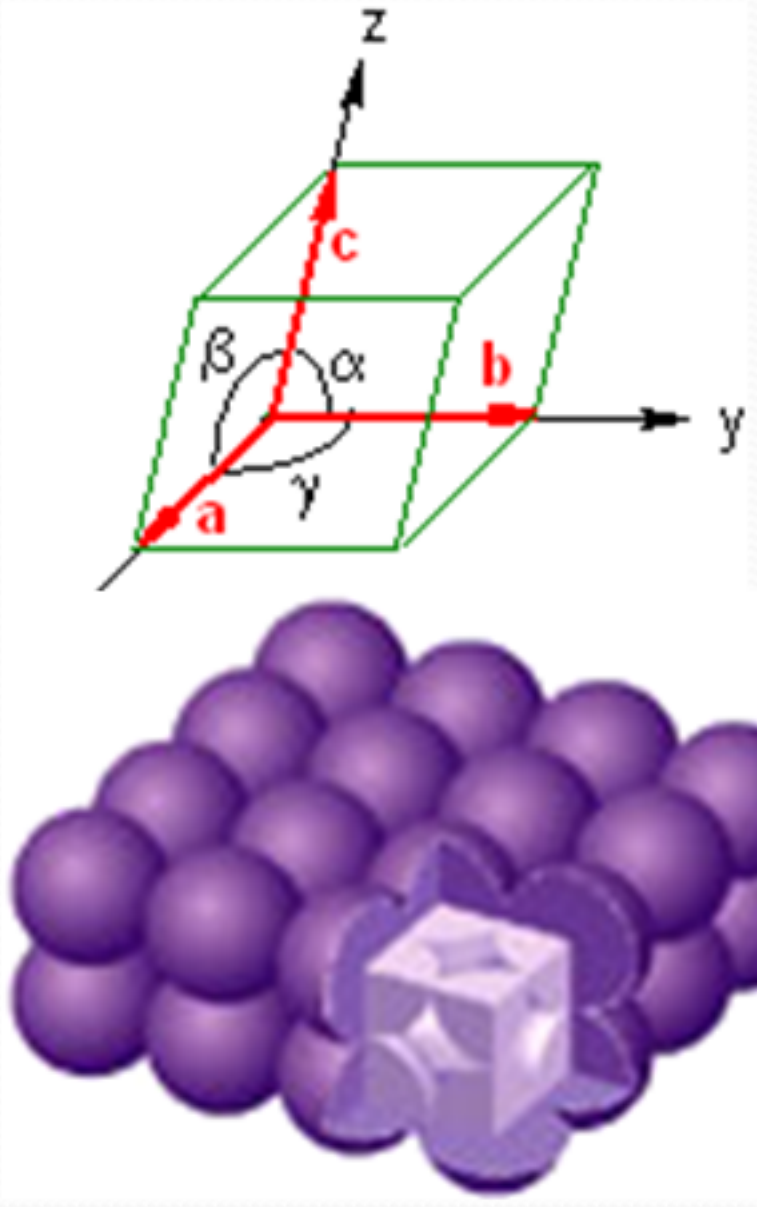
Primitive and conventional cells-hcp



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.

Coordination Number

- Coordination Number (CN) : The Bravais lattice points closest to a given point are the nearest neighbours.

- Because the Bravais lattice is periodic, all points have the same number of nearest neighbours or coordination number. It is a property of the lattice.

- A simple cubic has coordination number 6; a body-centered cubic lattice, 8; and a face-centered cubic lattice,12.

- Didalam kristal terdapat kisi-kisi yang ekivalen yang sesuai dengan lingkungannya dan diklasifisikan menurut simetri translasi.

  Operasi translasi kisi didefinisikan sebagai *perpindahan dari sebuah kristal oleh sebuah vektor translasi kristal* , maka persamaannya

$$\vec{T} = u_1\vec{a}_1 + u_2\vec{a}_2 + u_3\vec{a}_3$$

- Dimana u1,u2,u3 = bilangan bulat.
- a1, a2, a3 = vektor translasi primitive
- ≈ sumbu-sumbu kristal

✓ **Operasi Translasi Kisi :**

Perpindahan dari sebuah kristal oleh sebuah vektor translasi kristal

$$\vec{T} = u_1\vec{a}_1 + u_2\vec{a}_2 + u_3\vec{a}_3$$

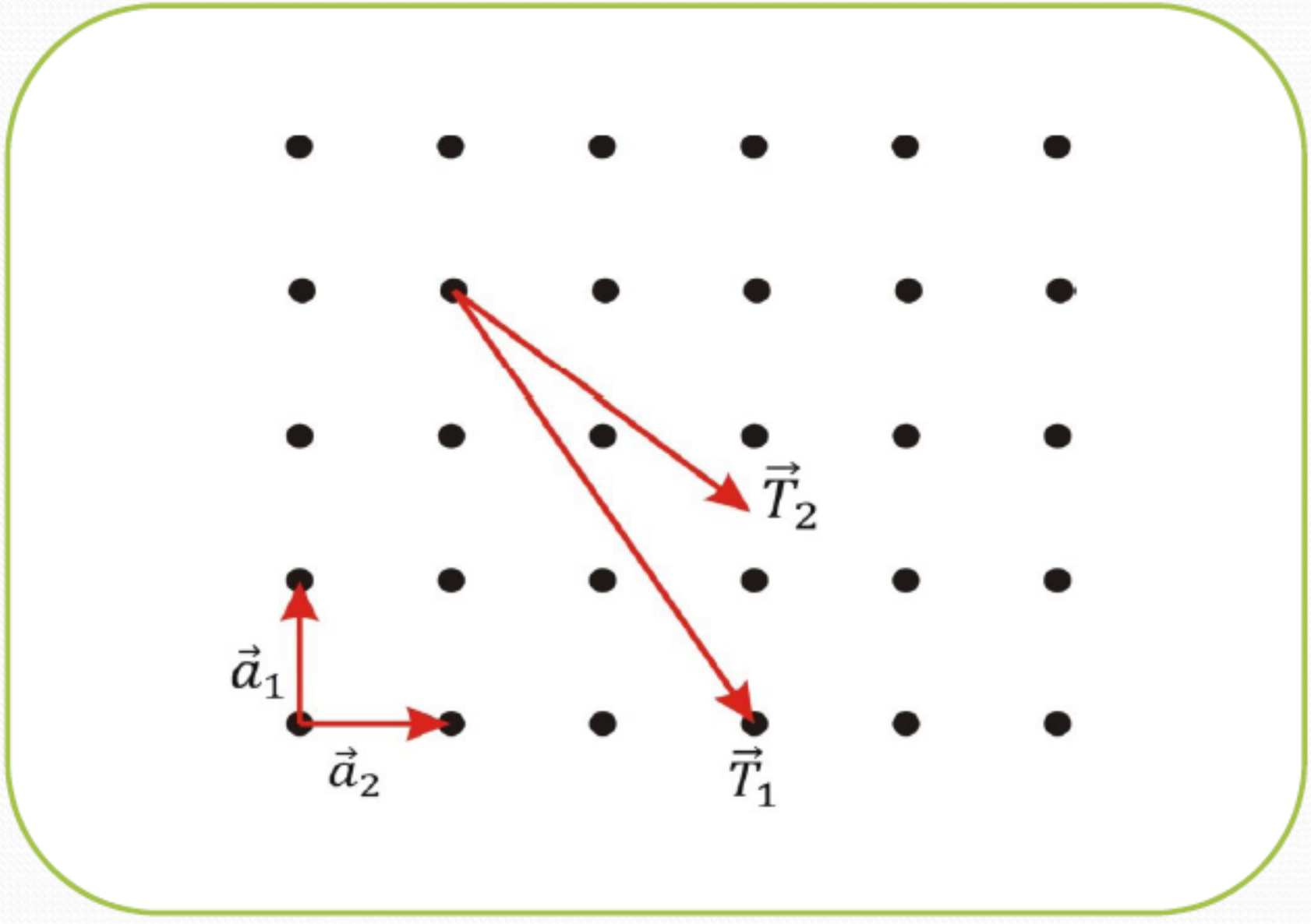
Keterangan :

$\vec{T}$ = vektor translasi kristal

u = Bilangan bulat

$\vec{a}$ = vektor translasi primitif/sumbu-sumbu kristal

Contoh Operasi Translasi Kisi



- **Untuk** $\vec{T}_1$

$$\vec{T}_1 = u_1\vec{a}_1 + u_2\vec{a}_2 + u_3\vec{a}_3$$

$$\vec{T}_1 = -3\vec{a}_1 + 2\vec{a}_2 + 0\vec{a}_3$$

$$\vec{T}_1 = -3\vec{a}_1 + 2\vec{a}_2$$

Jadi:

$u_1 = -3 \; dan \; u_2 = 2$

- **Untuk** $\vec{T}_2$

$$\vec{T}_2 = u_1\vec{a}_1 + u_2\vec{a}_2 + u_3\vec{a}_3$$

$$\vec{T}_1 = -1{,}5\,\vec{a}_1 + 1{,}5\,\vec{a}_2 + 0\vec{a}_3$$

$$\vec{T}_1 = -1{,}5\,\vec{a}_1 + 1{,}5\,\vec{a}_2$$

Jadi :

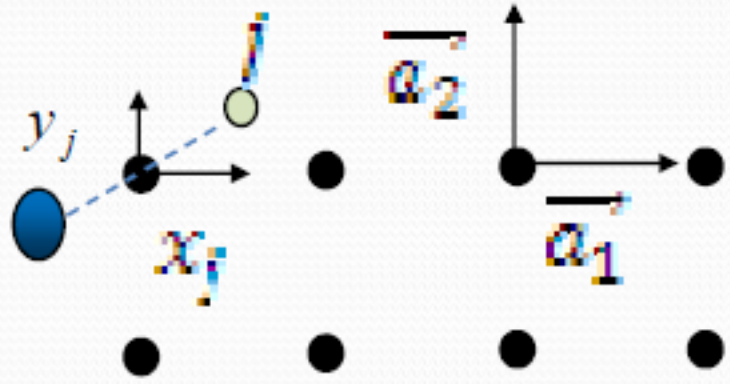
$u_1 = -1{,}5 \; dan \; u_2 = 1{,}5$

$\vec{T}_1$ **: vektor translasi (bilangan bulat)**

$\vec{T}_2$ **: bukan vektor translasi (bukan bilangan bulat)**

Posisi dari sebuah pusat atom *j* dari sebuah basis relatif terhadap titik latice dimana basis diletakkan adalah :

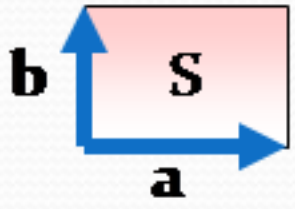
$$\overrightarrow{r_j} = x_j \overrightarrow{a_1} + y_j \overrightarrow{a_2} + z_j \overrightarrow{a_3}$$



Dimana : $0 \leq x_j, y_j, z_j \leq 1$

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