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.

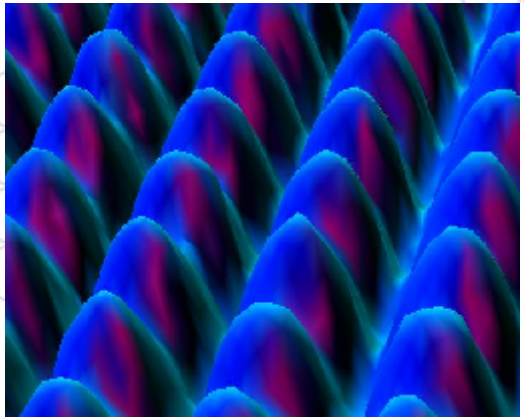
- We will concern in this course with solids with simple structures.

CRYSTAL LATTICE

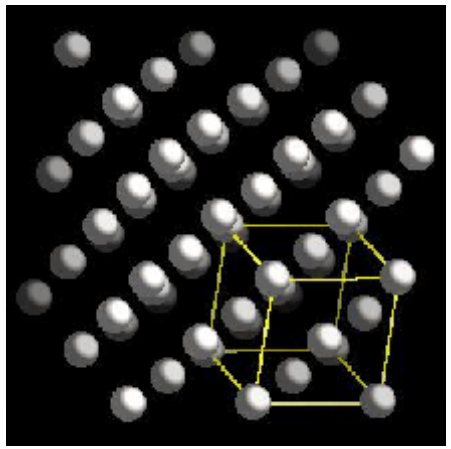
What is crystal (space) lattice?

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)



Crvstal lattice and
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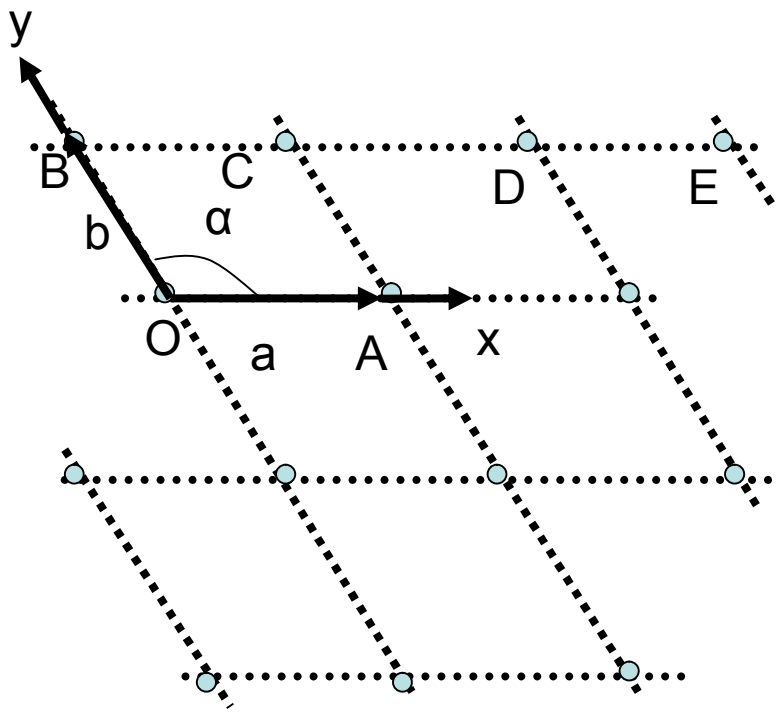
Crystal Lattice

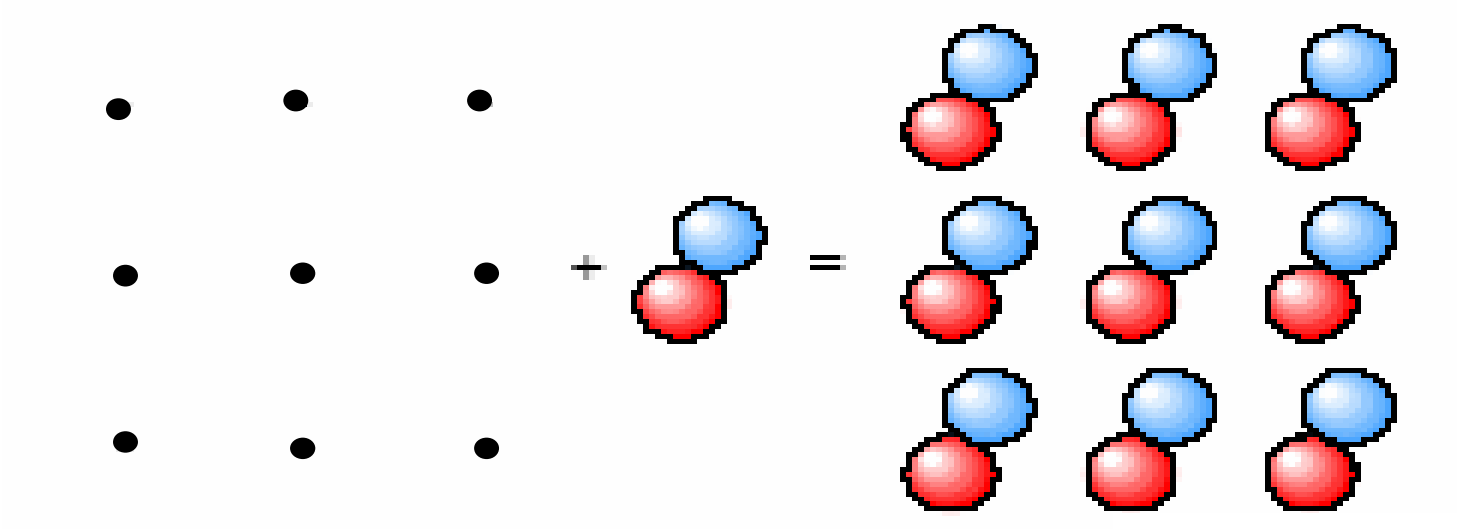
- An infinite array of points in space,
- Each point has identical surroundings to all others.
- Arrays are arranged exactly in a periodic manner.



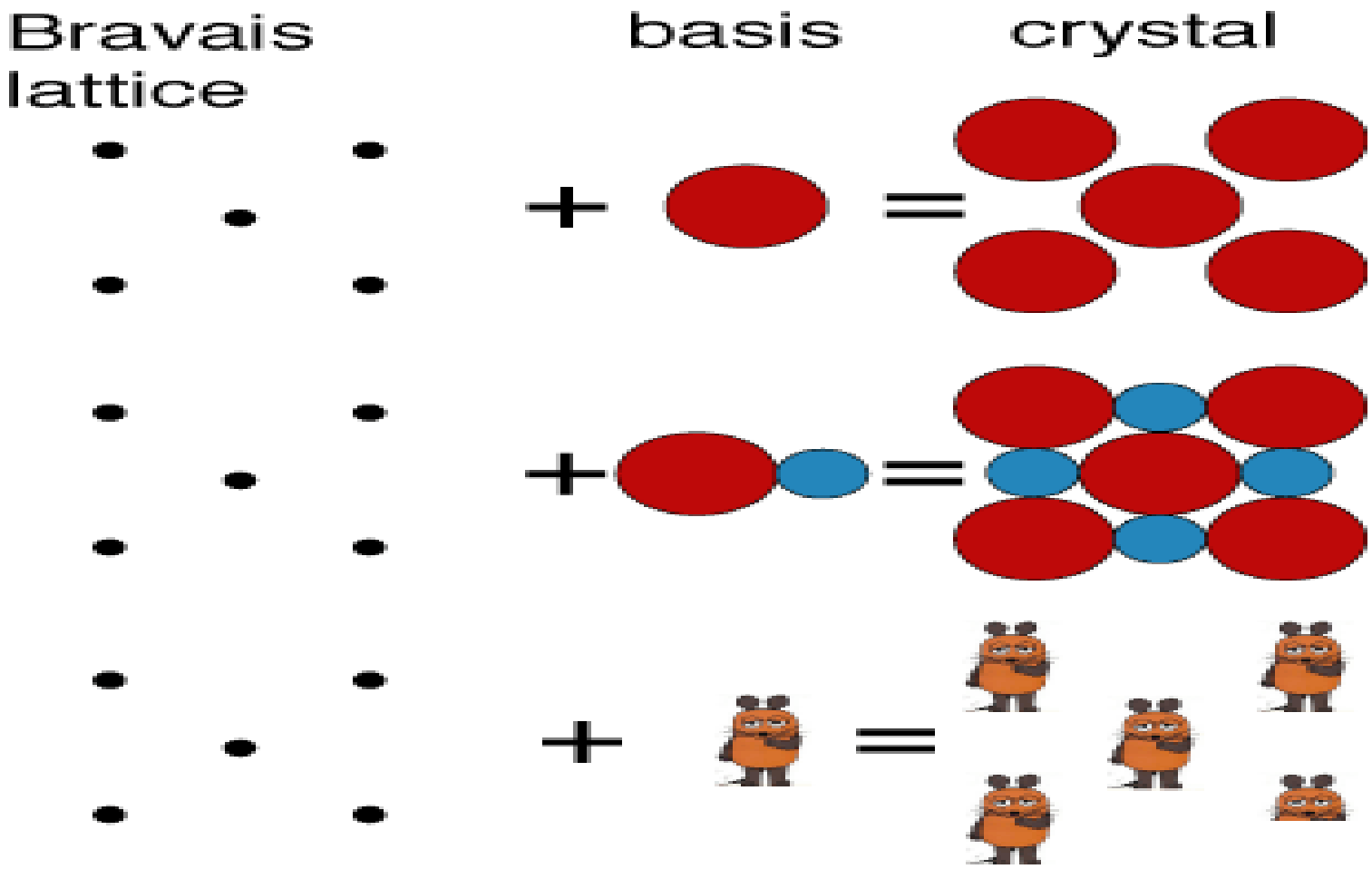
Crystal Structure

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

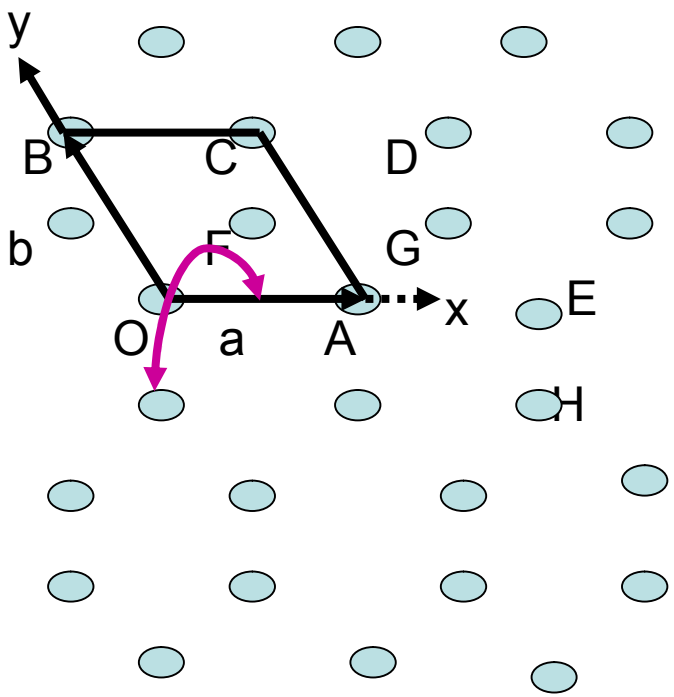


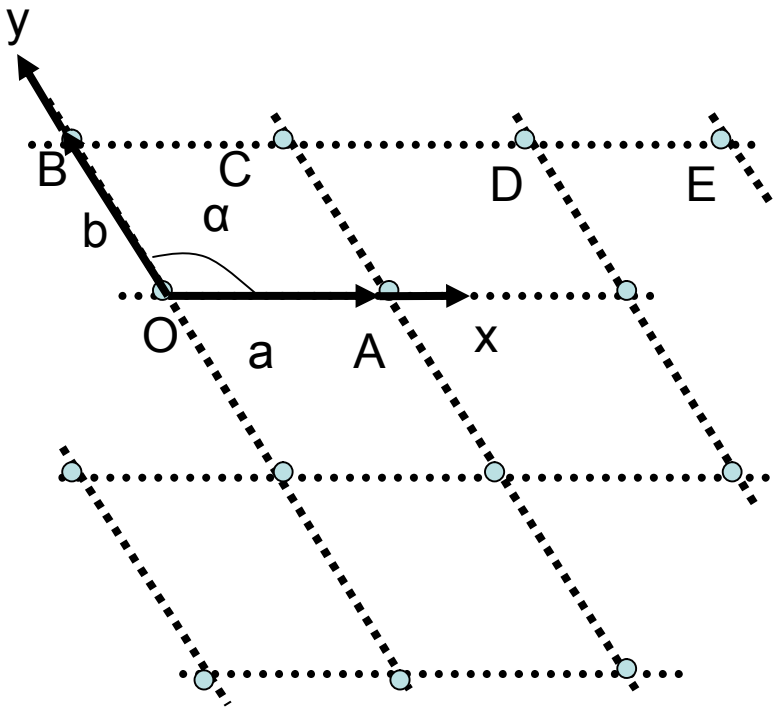
A two-dimensional Bravais lattice with different choices for the basis



Basis

- **A group of atoms which describe crystal structure**



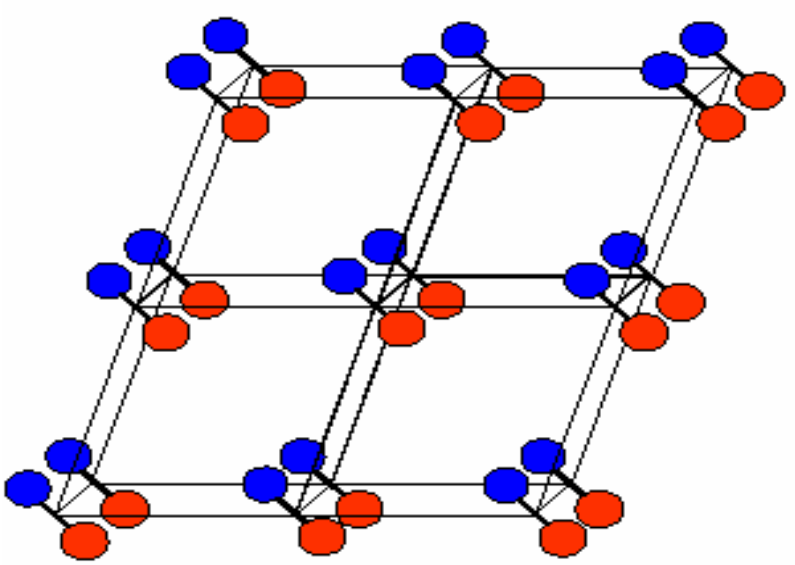


a) Situation of atoms at the corners of regular hexagons

b) Crystal lattice obtained by identifying all t

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

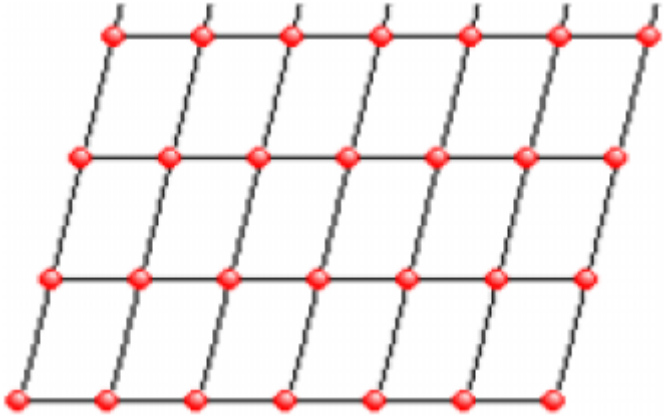


Crystal Structure = Crystal Lattice • + Basis

Crystal Lattice

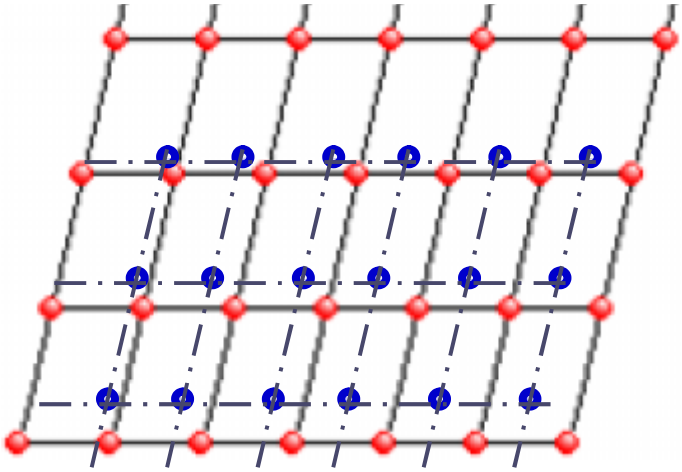
Bravais Lattice (BL)

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



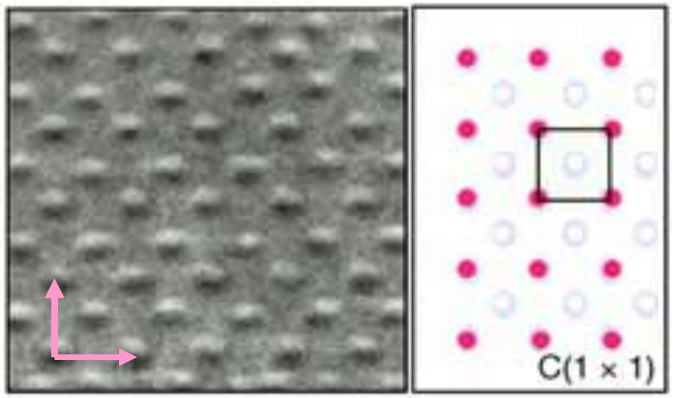
Non-Bravais Lattice (non-BL)

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



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

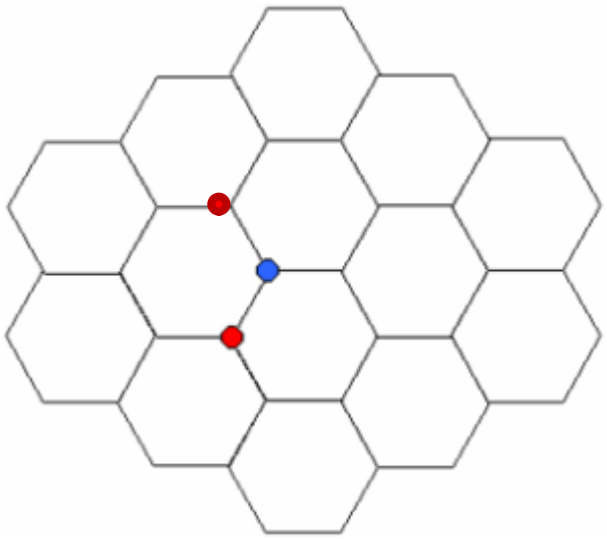
Types Of Crystal Lattices

2) Non-Bravais Lattice

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

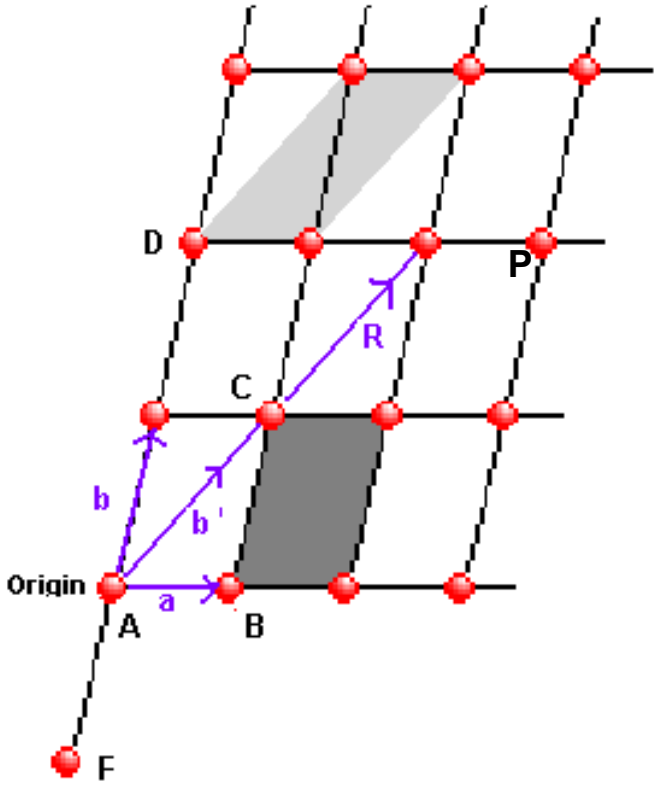
- The red side has a neighbour to its immediate left, the blue one instead has a neighbour to its right.
- Red (and blue) sides are equivalent and have the same appearance

-Red and blue sides are not equivalent. Same appearance can be obtained rotating blue side 180º.



Honeycomb

Translational Lattice Vectors – 2D



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

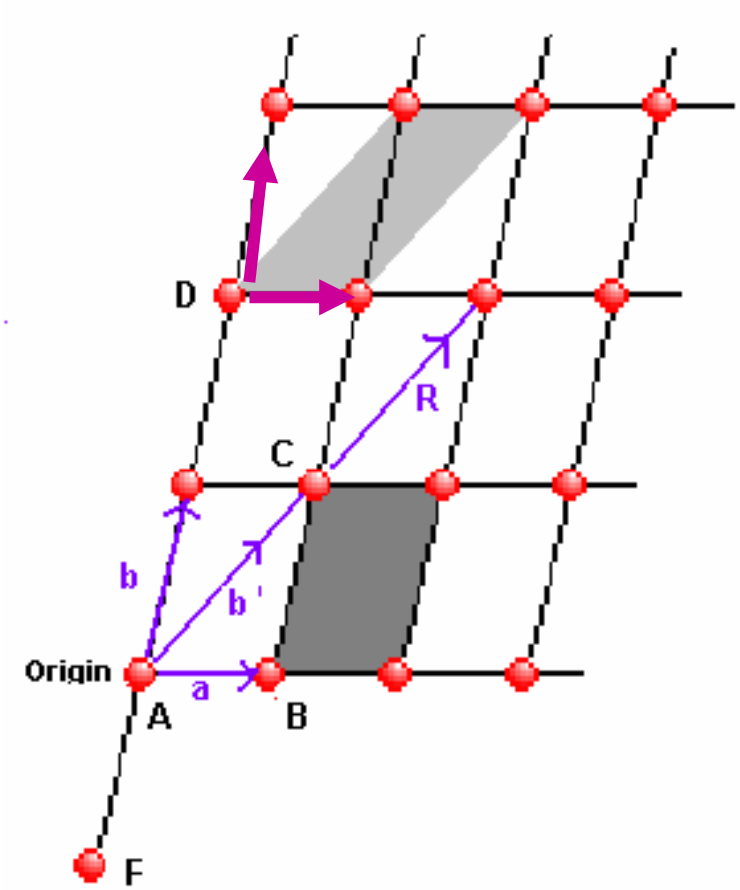
$$R_n = n_1\, a + n_2\, b$$

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.

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

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

Lattice Vectors – 2D

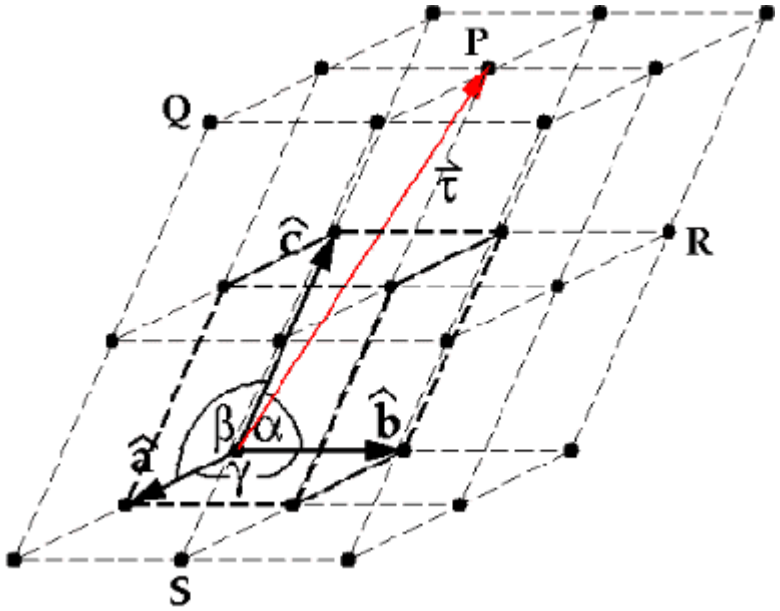


- The two vectors a and b form a set of lattice vectors for the lattice.

- The choice of lattice vectors is not unique. - Thus one could equally well take the vectors a and b' as a lattice vectors.

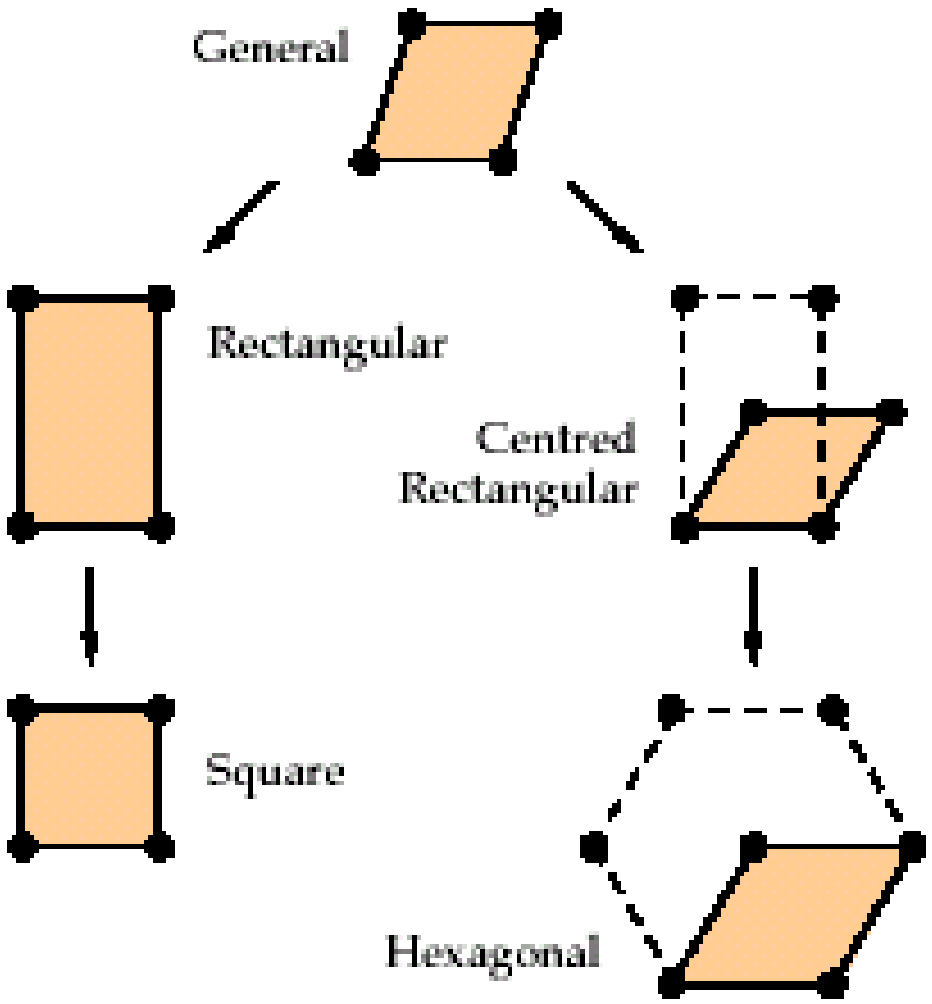
Lattice Vectors – 3D

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.



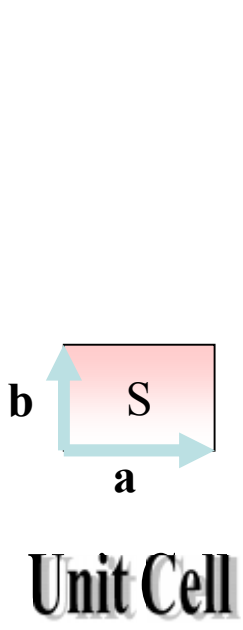
$$\mathbf{r'} = \mathbf{r} + u\,\mathbf{a} + v\,\mathbf{b} + w\,\mathbf{c} \qquad (1)$$

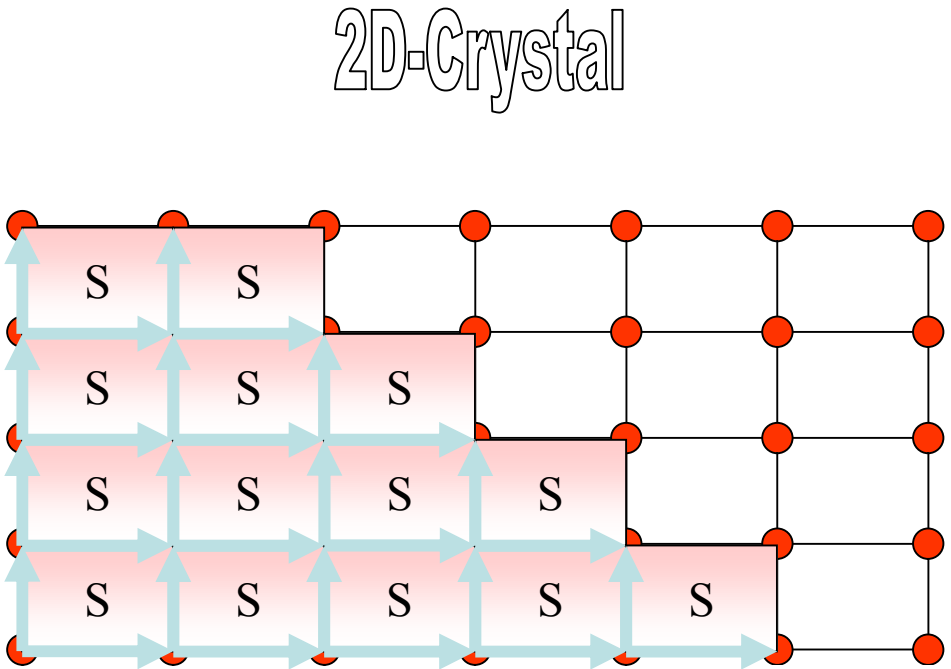
Five Bravais Lattices in 2D



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.

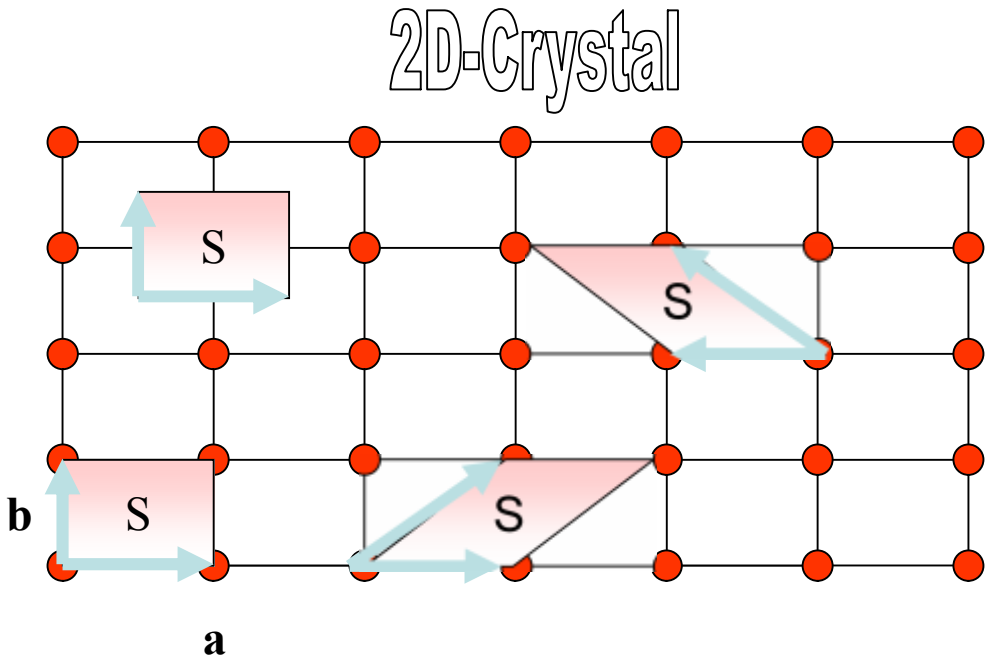




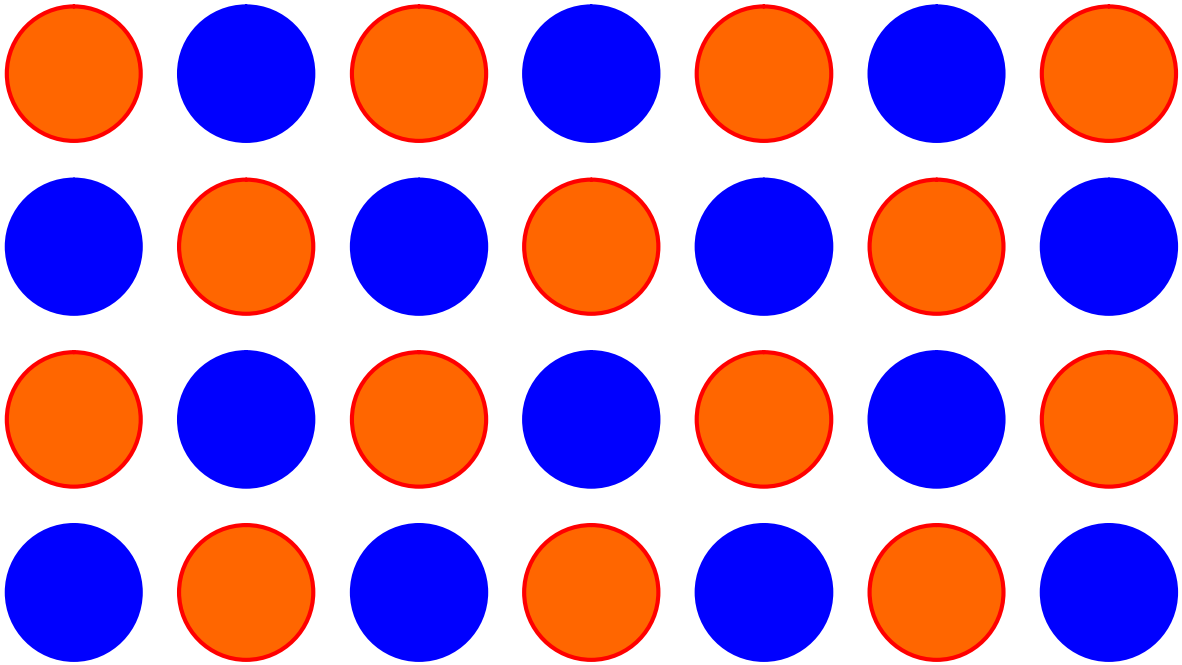
Unit Cell in 2D

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

The choice of unit cell is not unique.

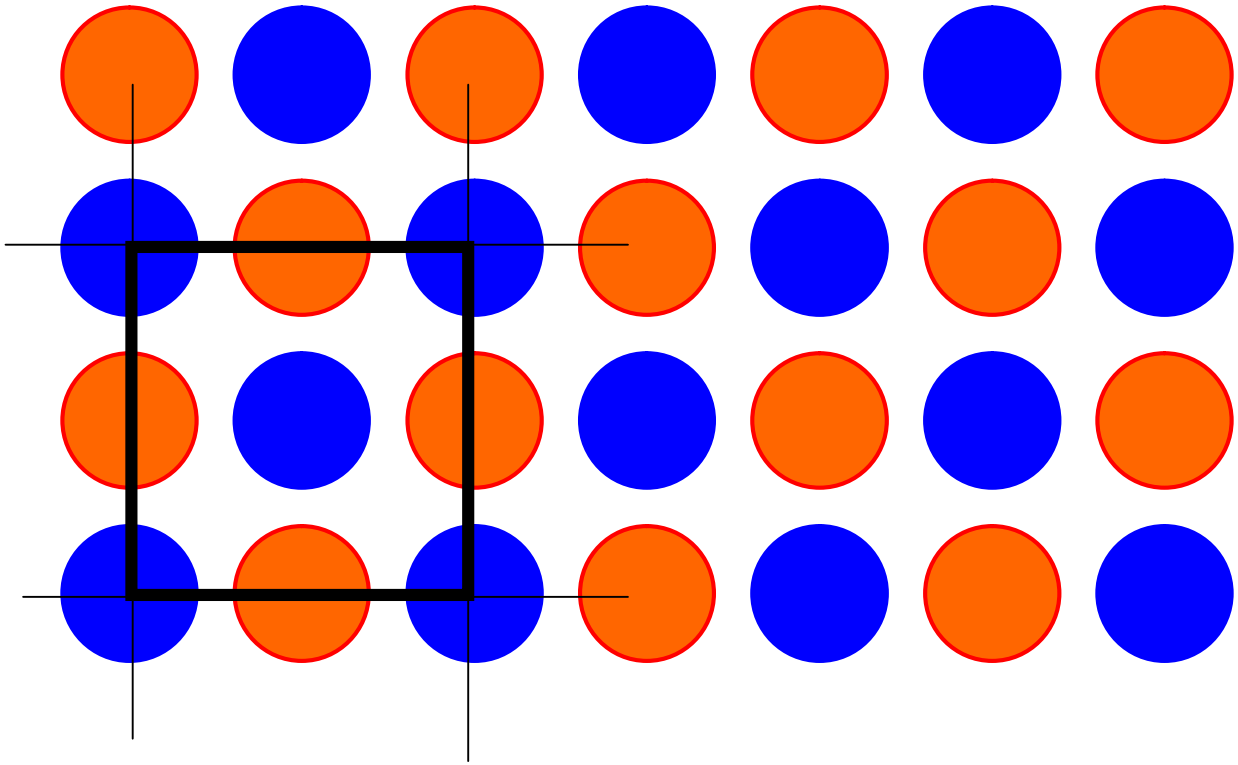


2D Unit Cell example -(NaCl)

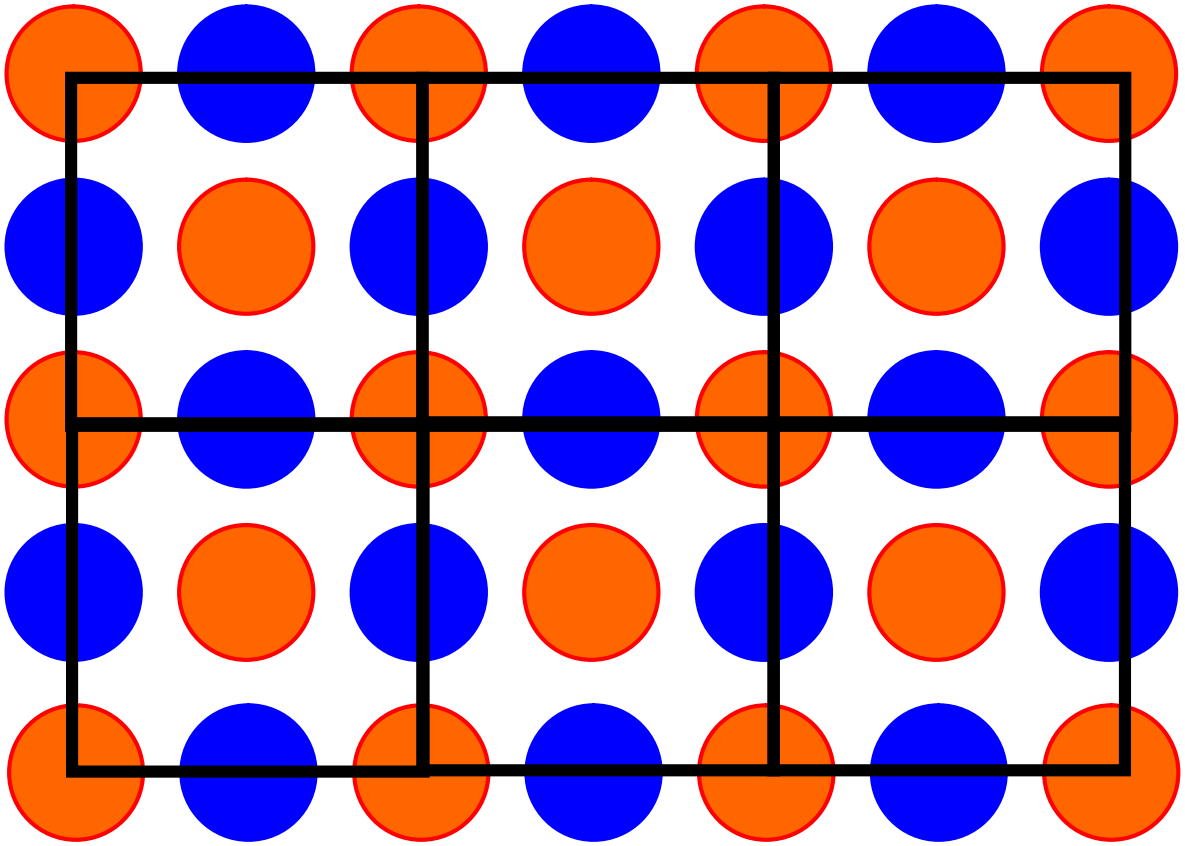


We define **lattice points** ; these are points with *identical environments*

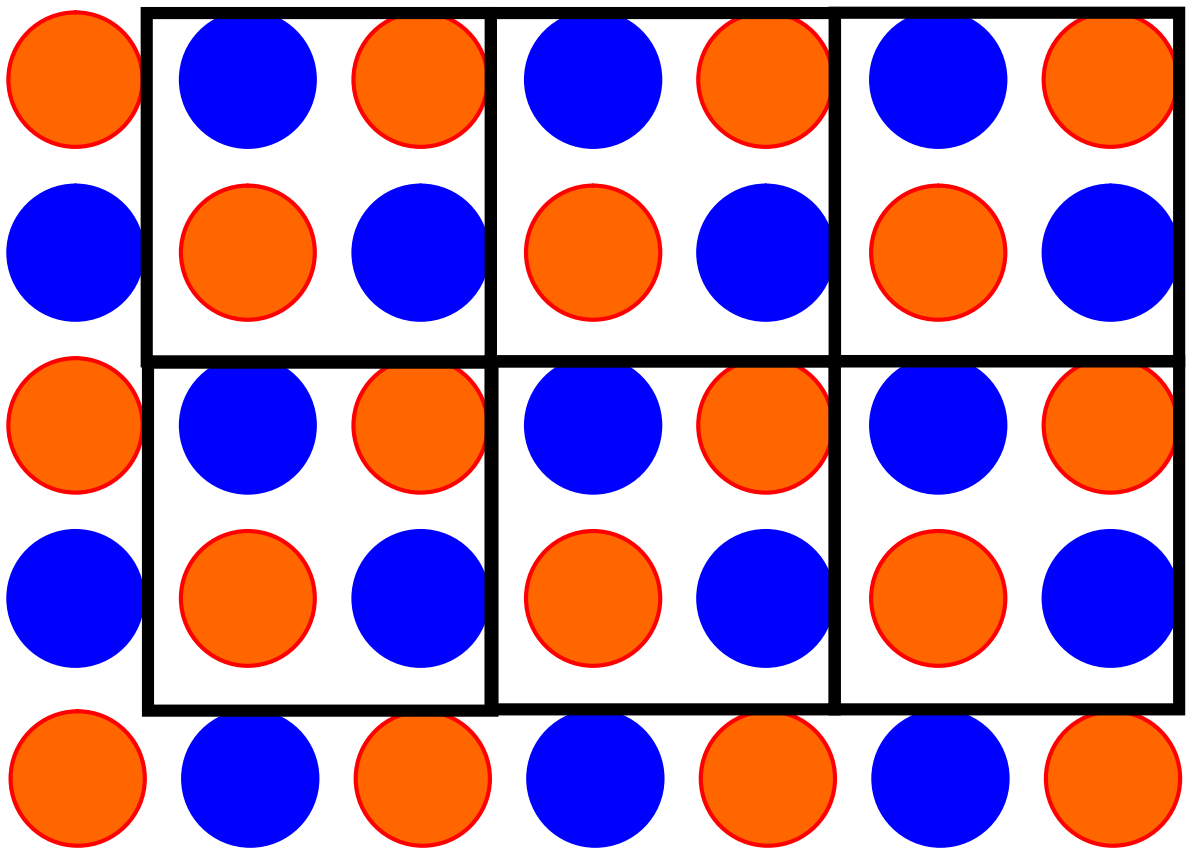
Choice of origin is arbitrary - lattice points need not be atoms - **but** unit cell size should always be the same.



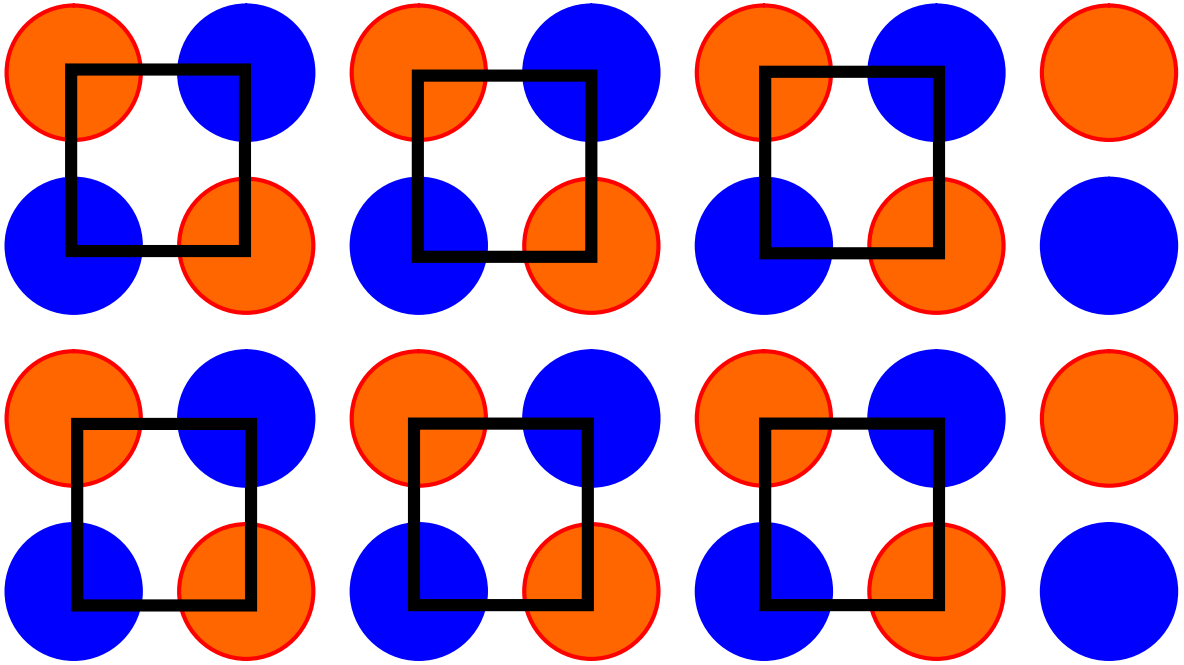
This is also a unit cell -
it doesn't matter if you start from Na or Cl



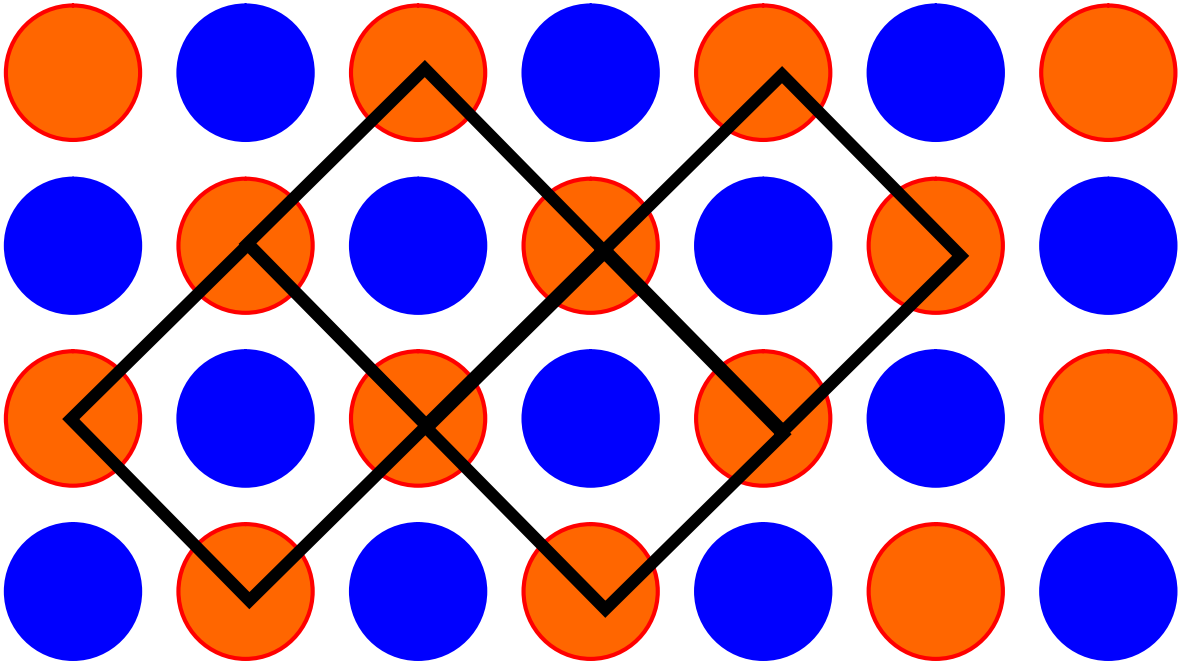
- or if you don't start from an atom



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



In 2D, this IS a unit cell
In 3D, it is NOT



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