Crystal Structure

CRYSTALS

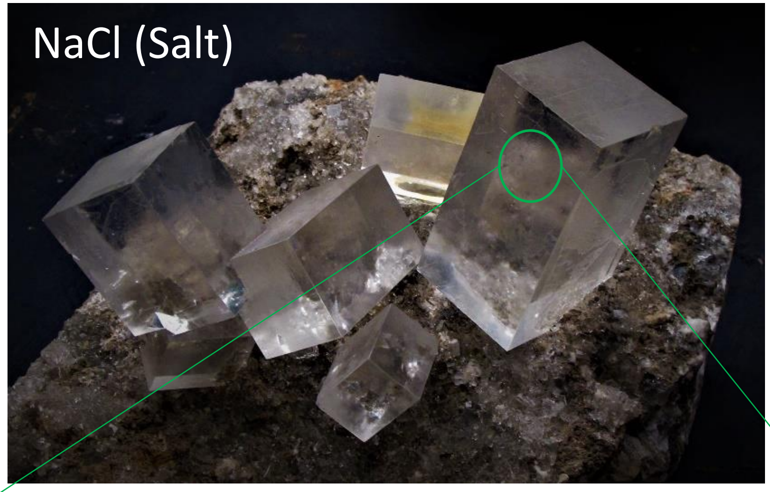

NaCl (Salt)

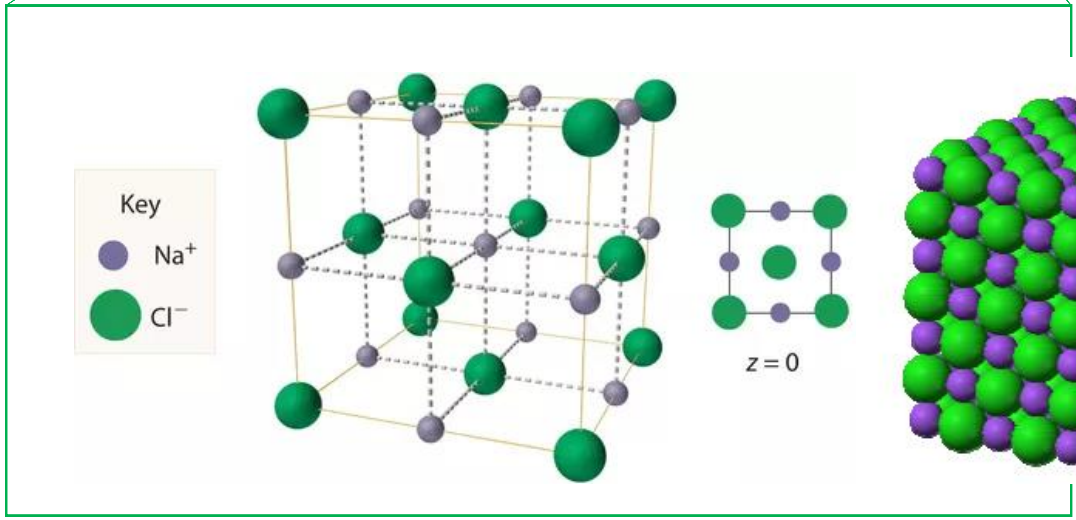

C (Diamond)


SiO_2 (Quartz)

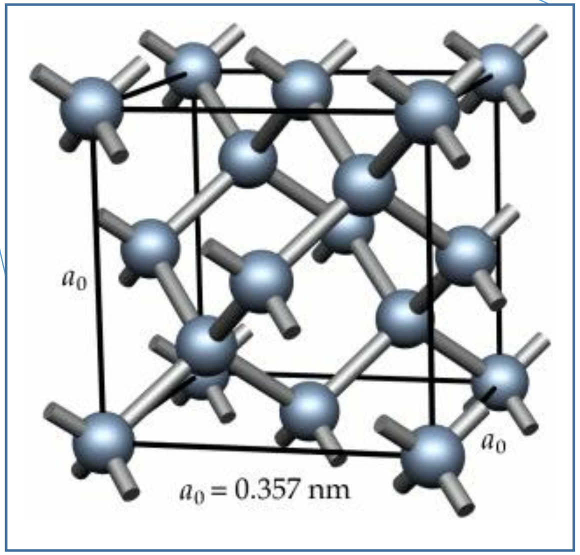

$YBa_2Cu_3O_{7-x}$ (superconductor)

A **crystal** is a periodic array of atoms or group of atoms



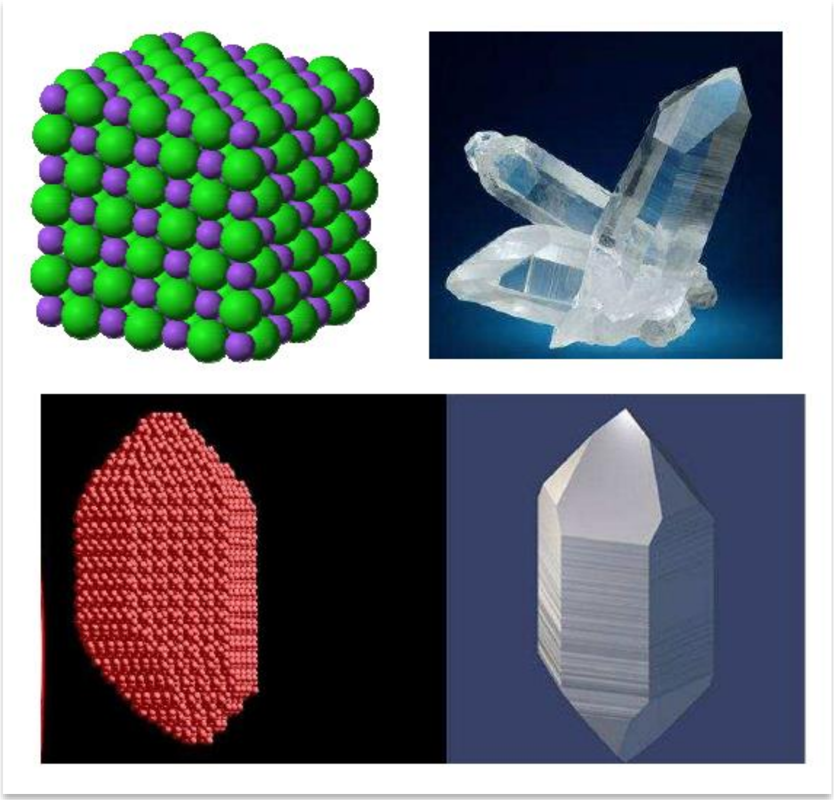


C (Diamond)

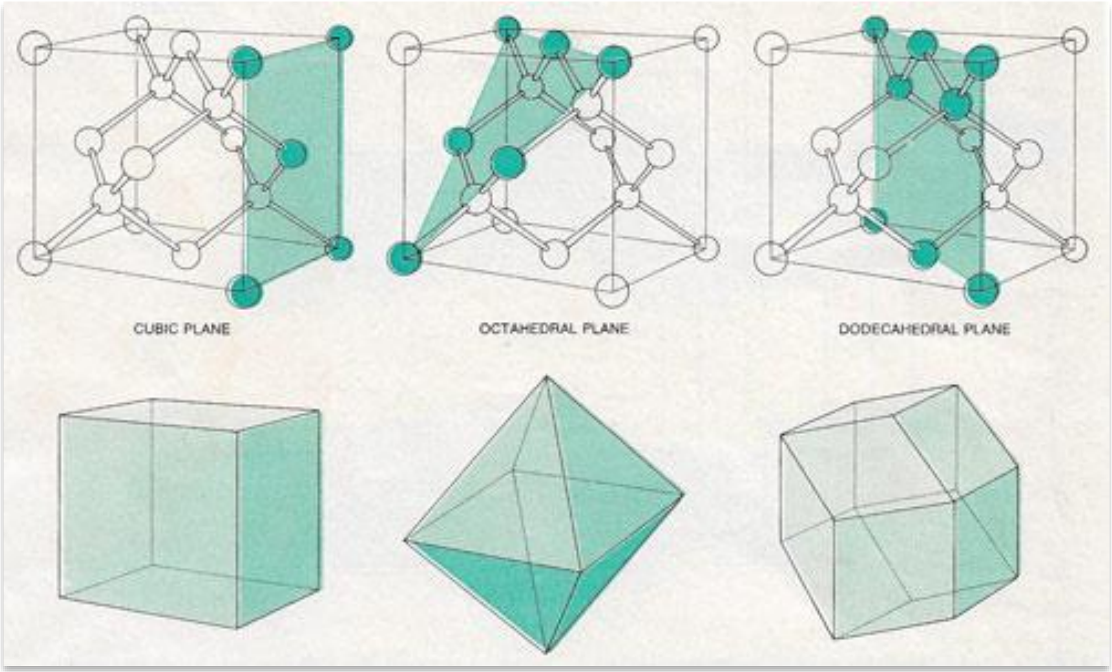


A **crystal** is a periodic array of atoms or group of atoms

NaCl (Salt)



C (Diamond)

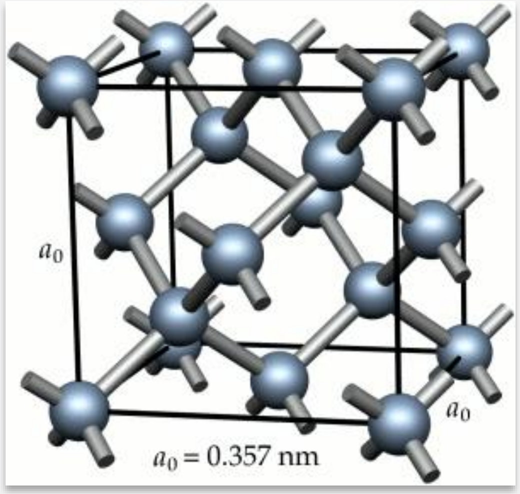


The macroscopic morphology of a crystal reflects its underlying structure

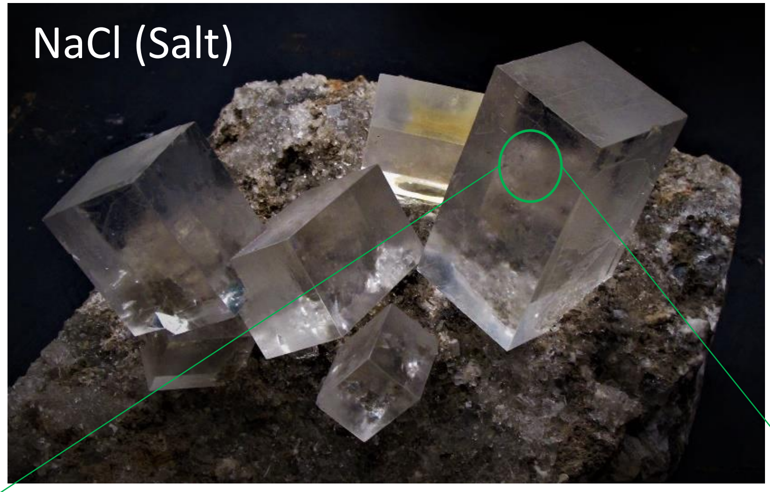
Learning outcomes of the lecture

- **Describe a crystal structure**

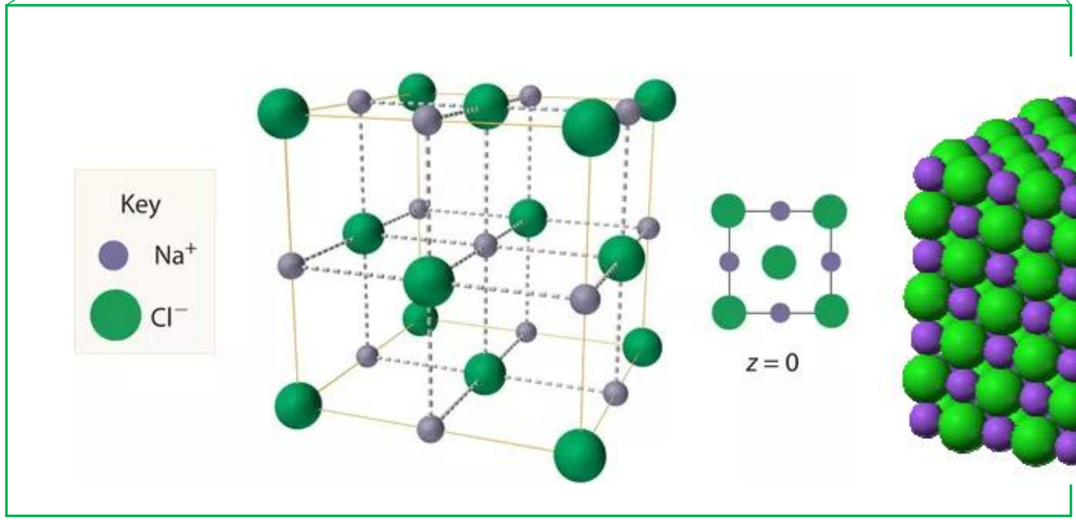
1. the Lattice

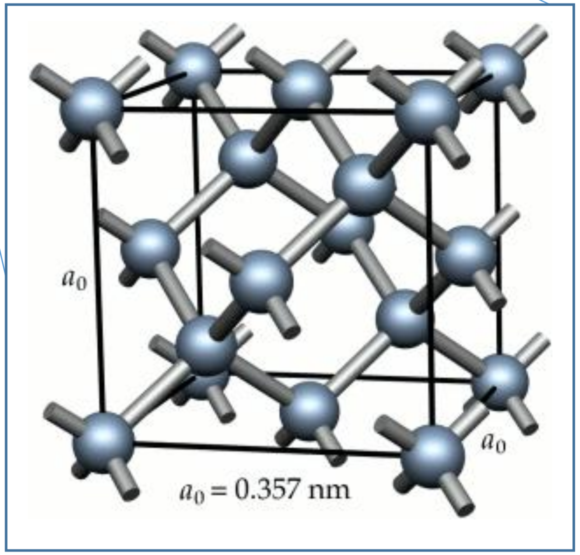


A **crystal** is a periodic array of atoms or group of atoms



Diamond (C)



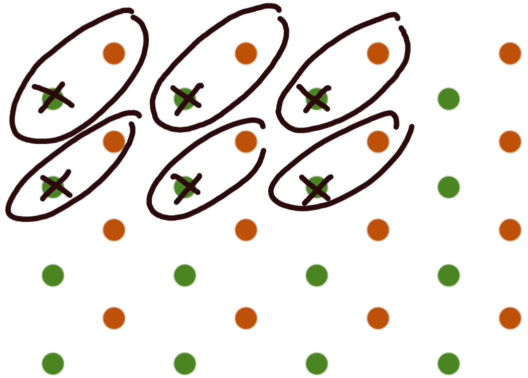


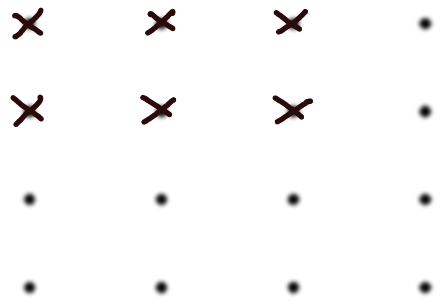
another definition

A **crystal** consists of a repeating pattern of objects (i.e. atoms or molecules) in an effectively infinite 3D array

A convenient way of describing a crystal:

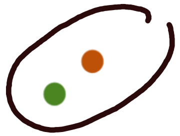
Crystal	=	**Lattice**	+	**Basis**





Lattice of points
(Bravais Lattice)

(set of mathematical points)



Basis of atoms

(physical object "attached" to the lattice point)

Lattice

- Infinite array of points in the space, in which each point has identical surroundings to all other points

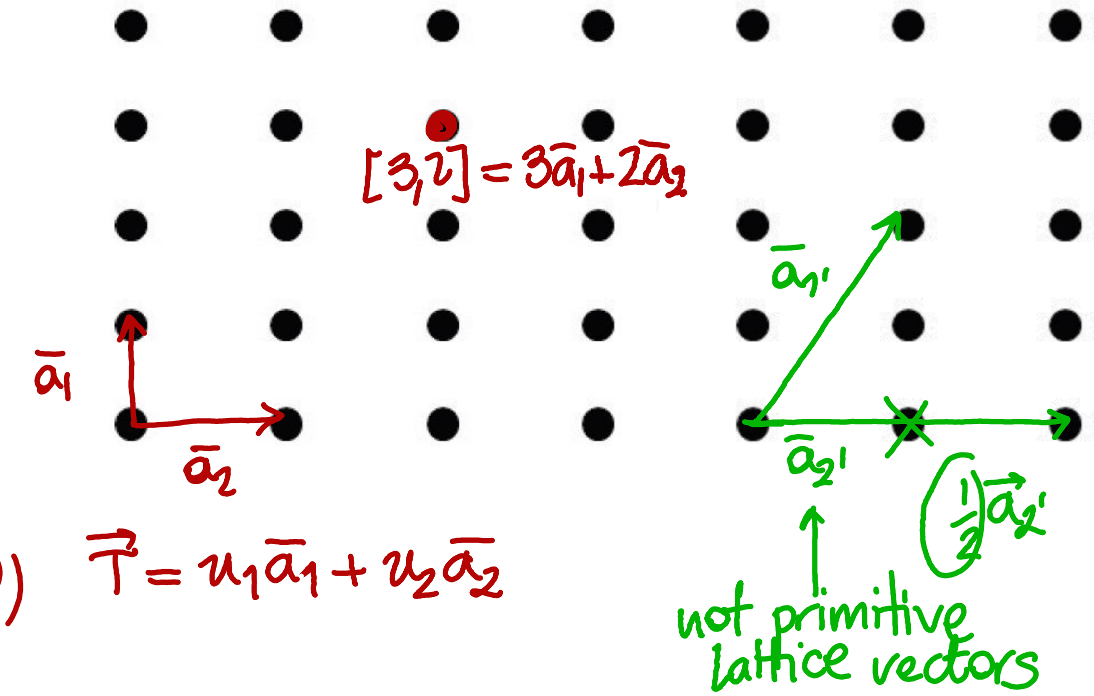
Lattice points are generated by translation vectors:

$$\vec{r}' = \vec{r} + \vec{T}$$

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

with $\bar{a}_i$: primitive lattice vectors

u_i : arbitrary integers



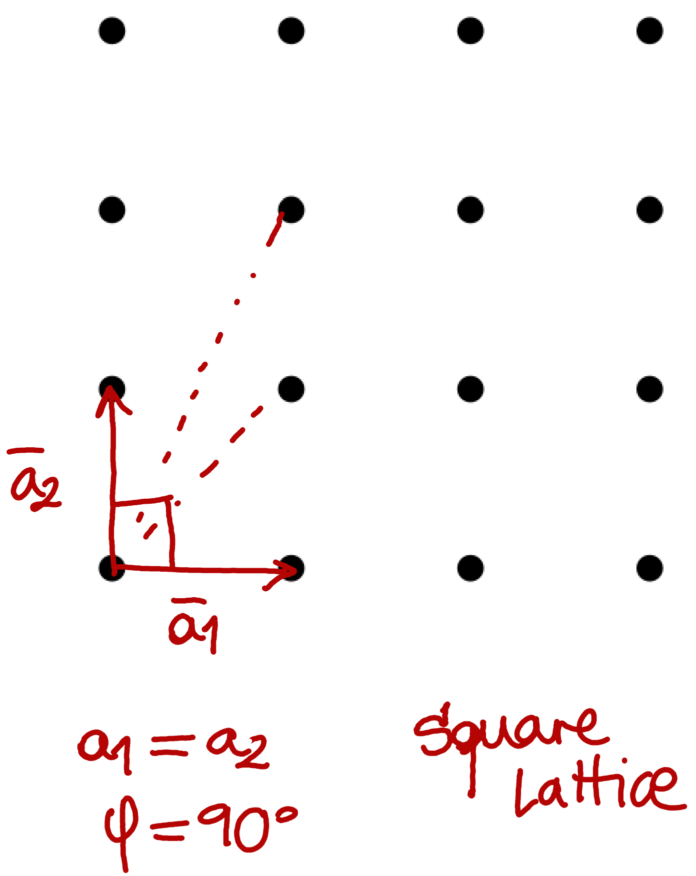
2D) $\vec{T} = u_1\bar{a}_1 + u_2\bar{a}_2$

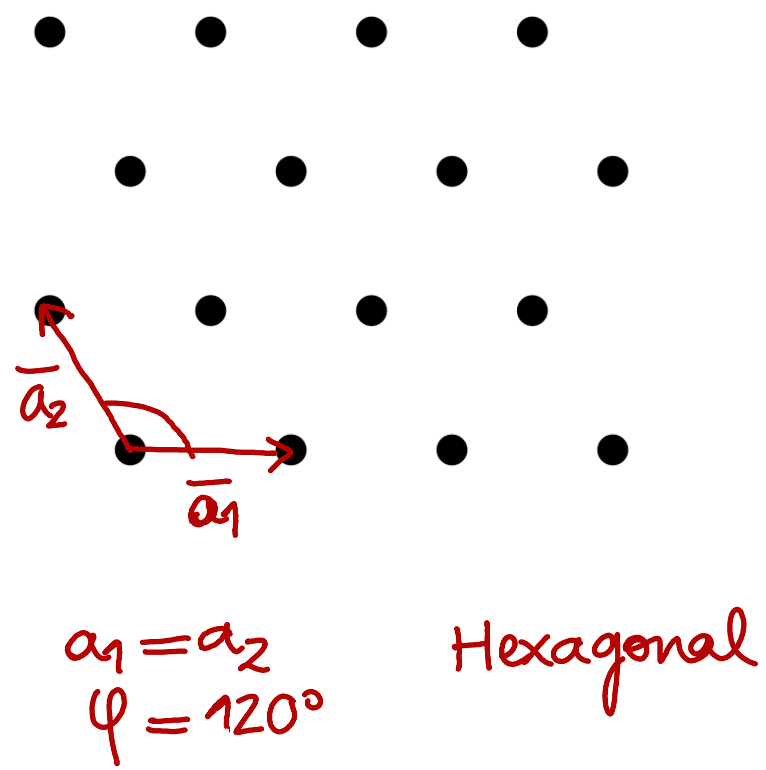
property, i.e. electronic density

$$\rho(\vec{r}) = \rho(\vec{r} + \vec{T})$$

Alternative definition: A **lattice** is an infinite set of points defined by the integer sum of a set of linearly independent primitive lattice vectors

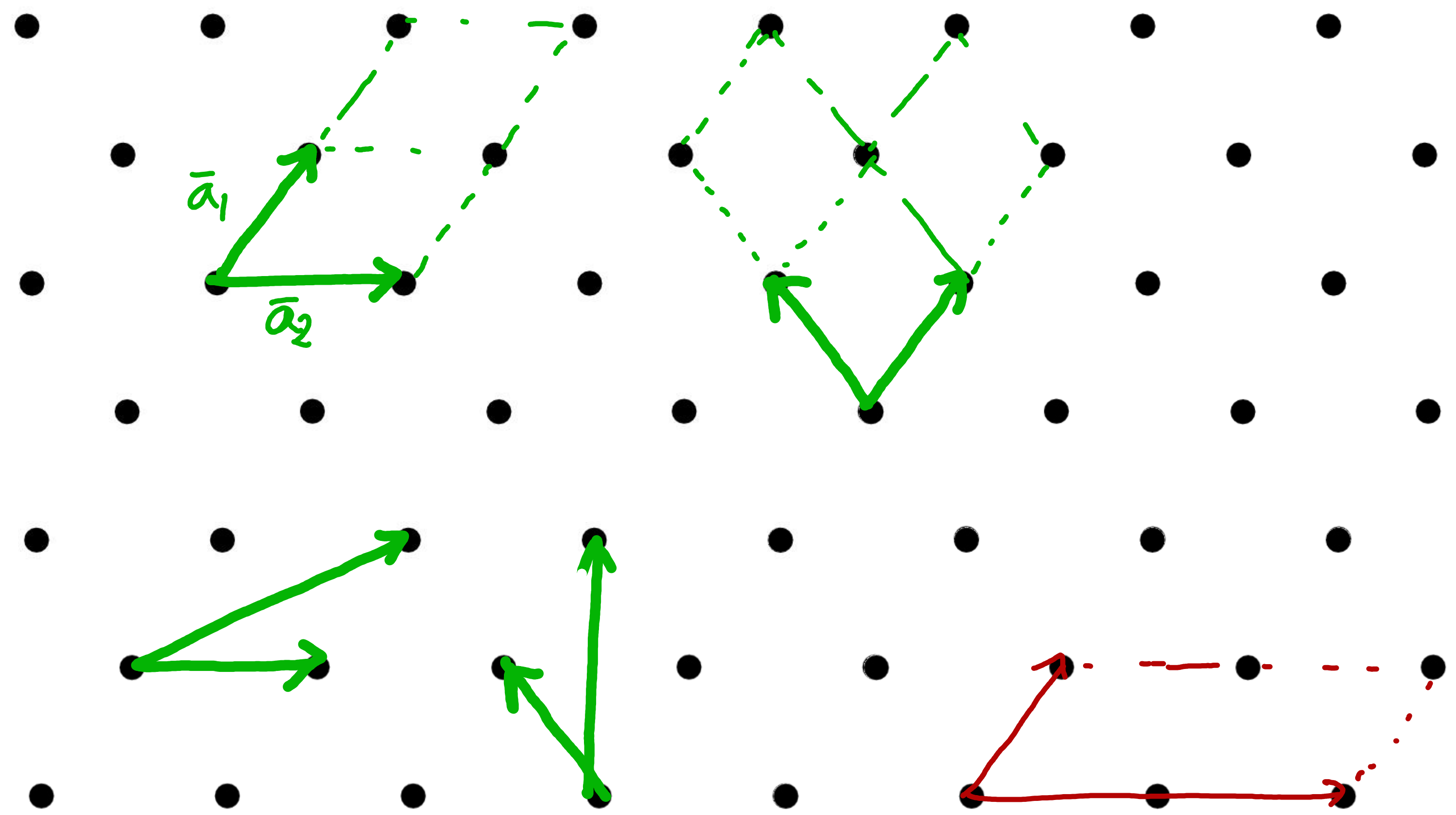
If all the points of the lattice, and only the lattice points, can be reached with n_i integers, the $\bar{a}_i$ are called <u>primitive lattice vectors</u>





Is the choice of primitive lattice vectors unique? NO!

$$\vec{T} = n_1 \bar{a}_1 + n_2 \bar{a}_2$$



All valid sets of possible primitive lattice vectors

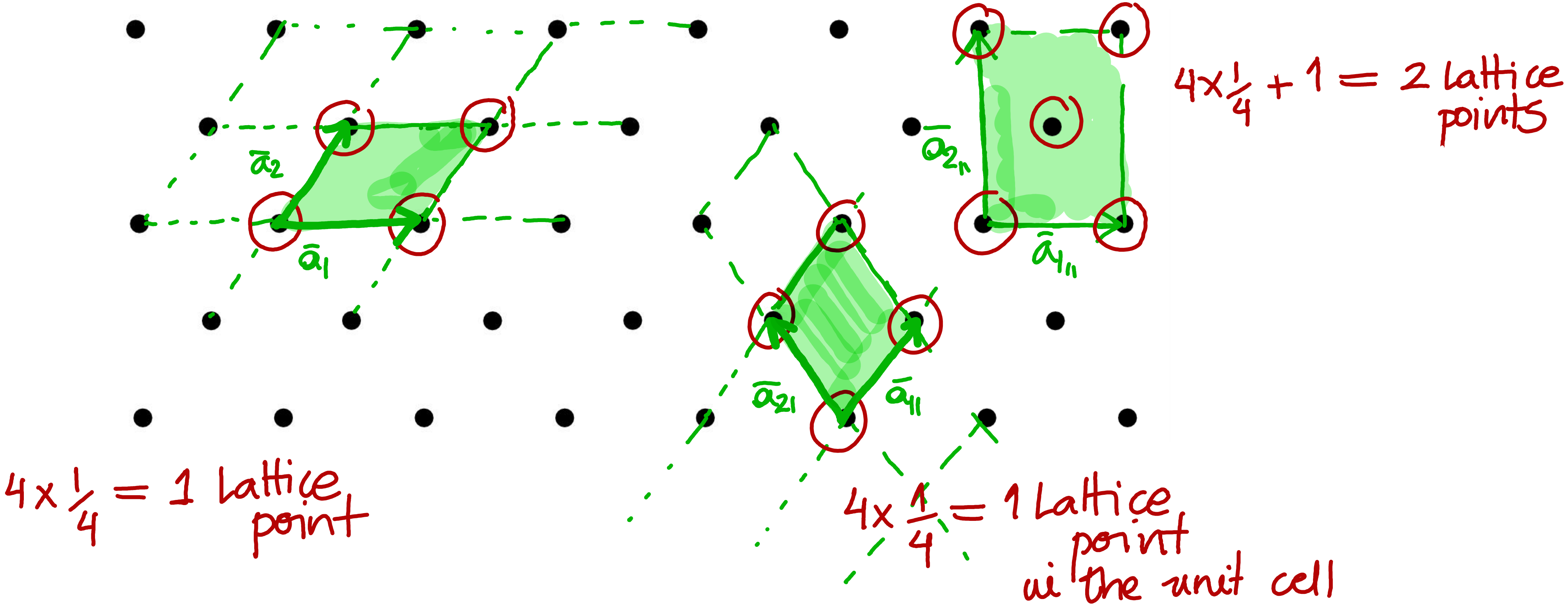
Not primitive translation vectors

in 1D): yes!

Unit cell

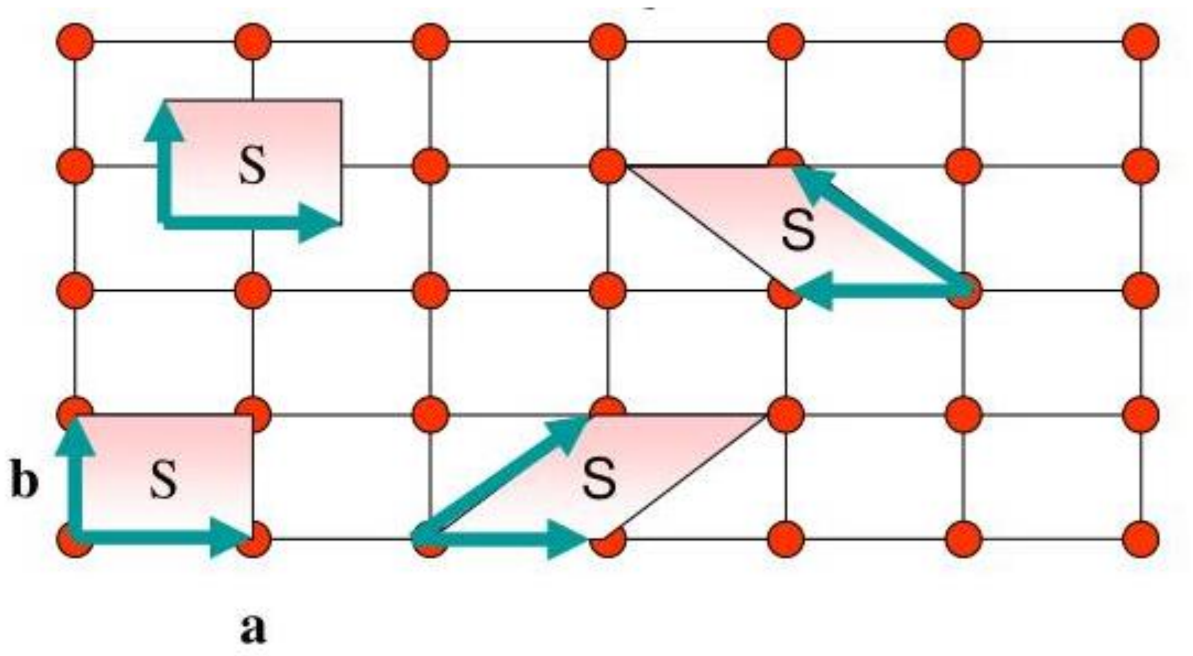
- A unit cell is a region of space that when repeated completly fills all of space and reconstructs the full structure

Equivalently: "the repeated motif which is the element building block of the periodic structure"



Primitive Unit Cell

- A **primitive unit cell** for a periodic crystal is a unit cell containing exactly one lattice point

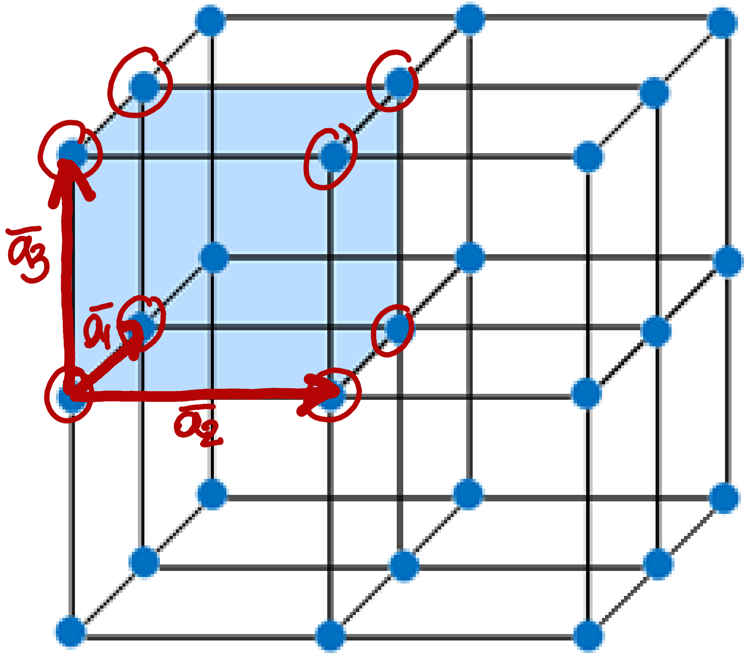


- there is no cell of smallest volume than $|\bar{a}_1 \cdot \bar{a}_2 \times \bar{a}_3|$

Primitive unit cell is not unique!

Primitive Unit Cell in 3D

$8 \times \frac{1}{8} = 1$ Lattice point per primitive cell



Primitive unit cell in 3D

<u>Wigner-Seitz</u> method for definig a primitive unit cell

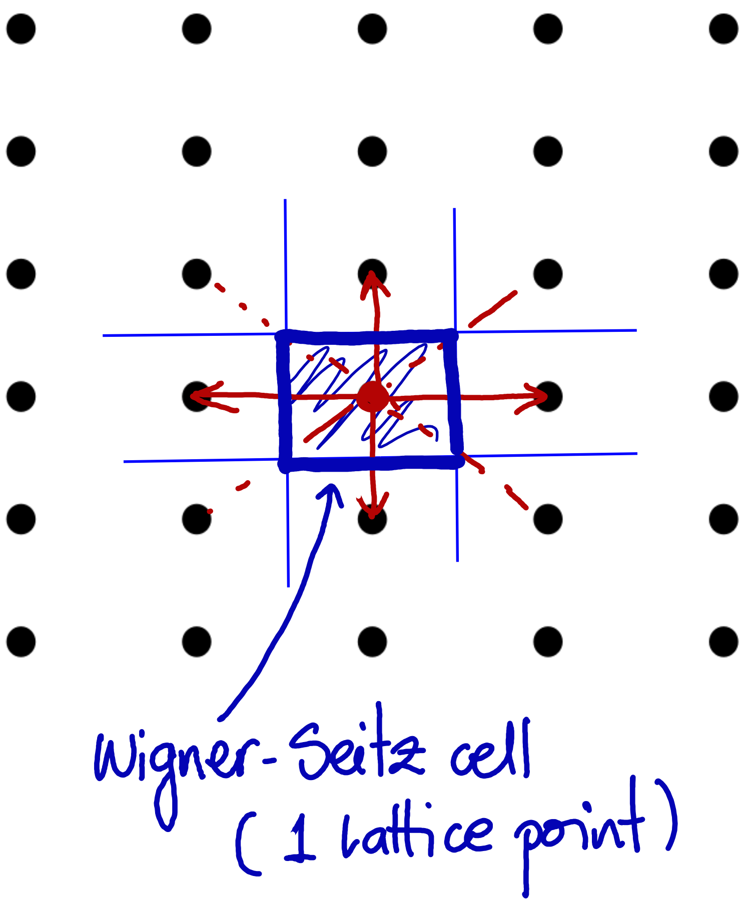
1. Choose a lattice point.

2. Construct vector to connect this point to all neighboring lattice points.

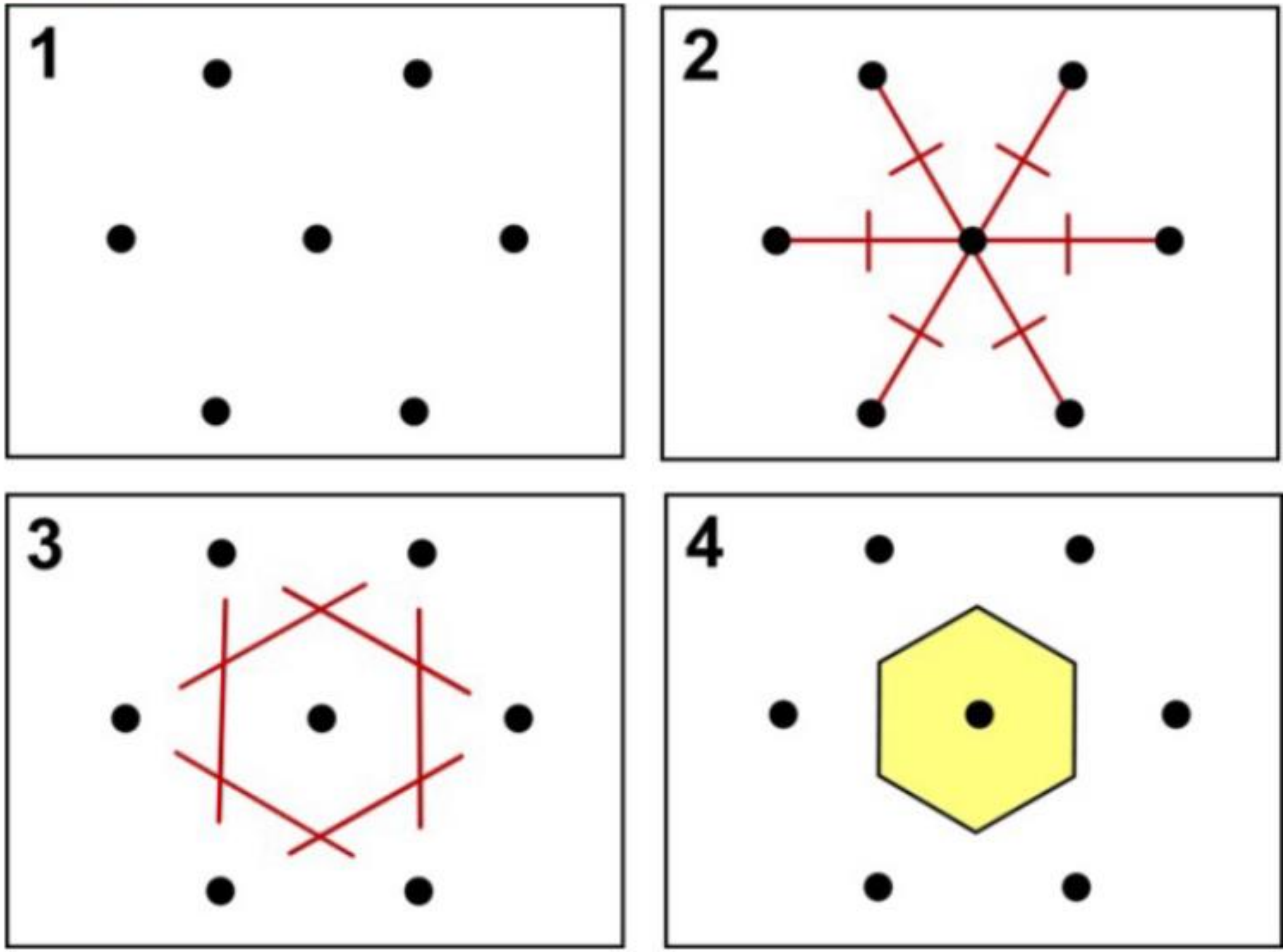
3. Planes are then constructed perpendicular to and passing through midpoints of these vectors

⬇

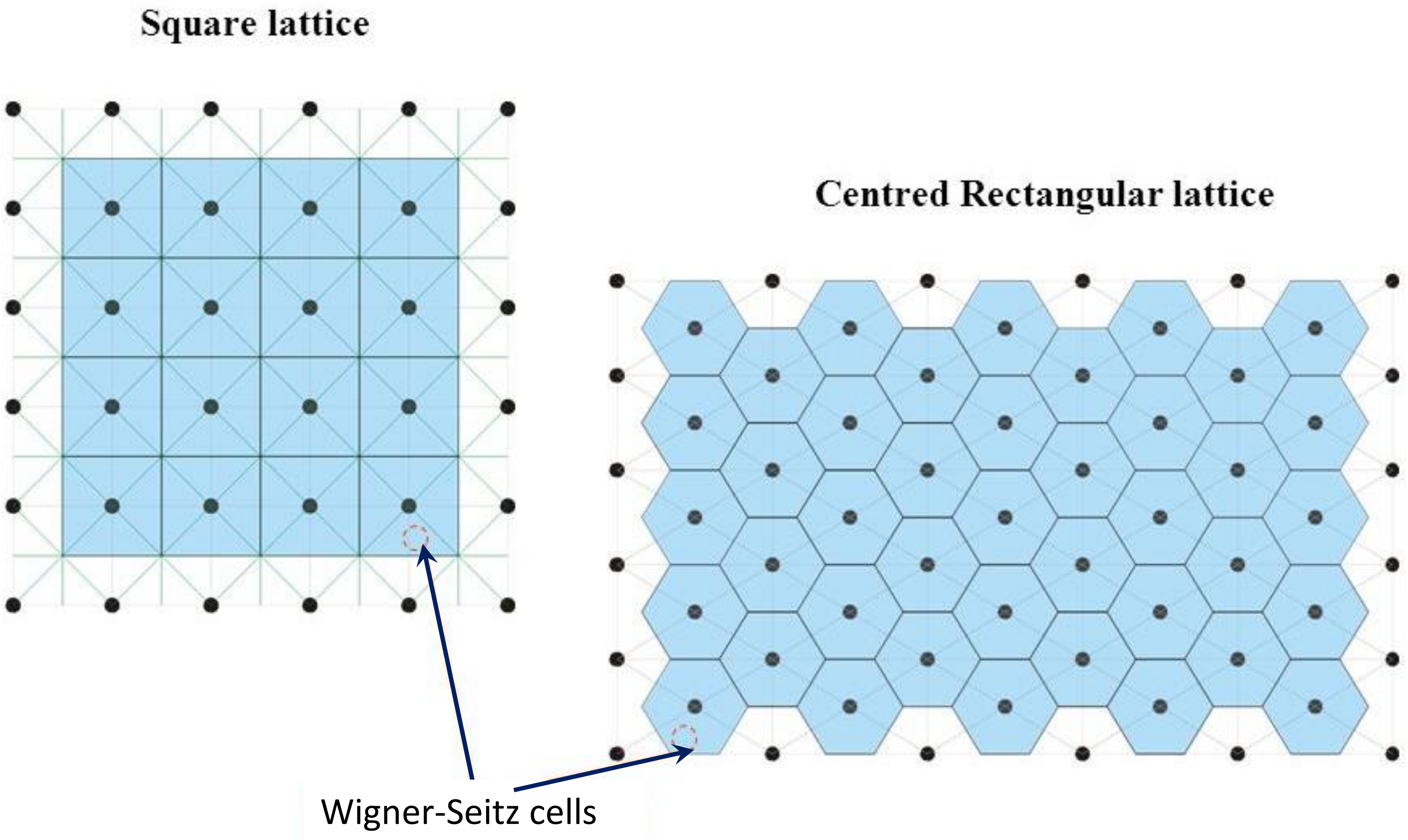
The smallest volume enclosed is called as a Wigner-Seitz cell.



Wigner-Seitz construction



Wigner-Seitz cells



Quiz: Which are primitive unit cells of the lattice?