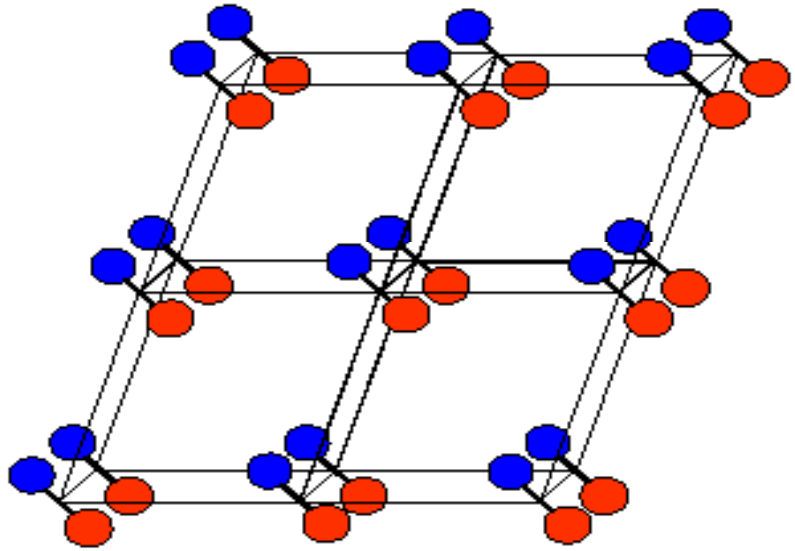
Crystal structure

- 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

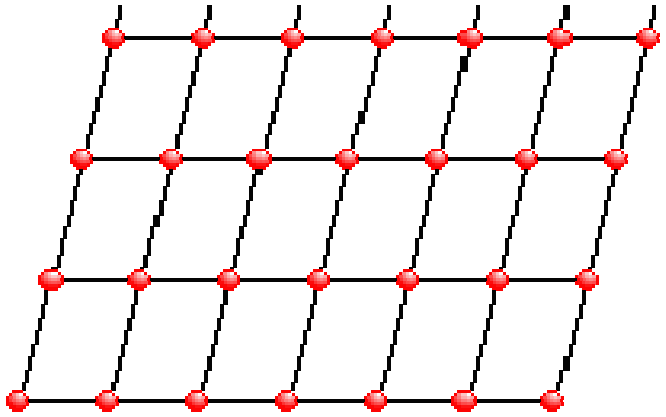
Crystal Lattice

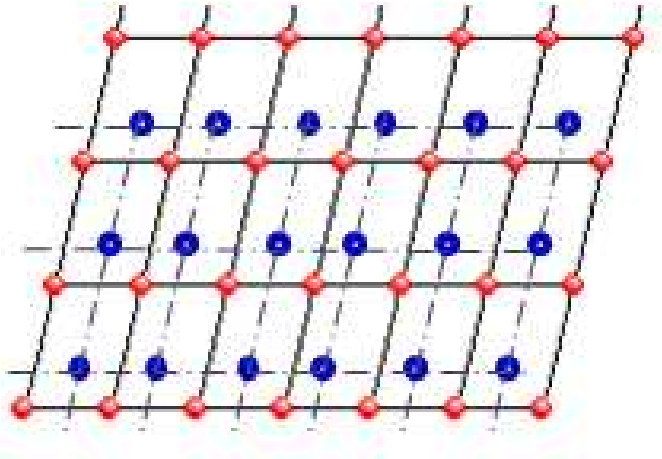
Bravais Lattice (BL)

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

Non-Bravais Lattice (non-BL)

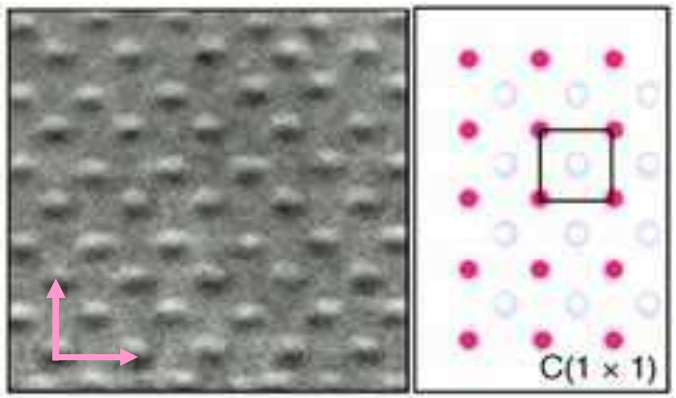
- Atoms can be of different kind
- Some lattice points are not equivalent
- A combination of two or more BL





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.

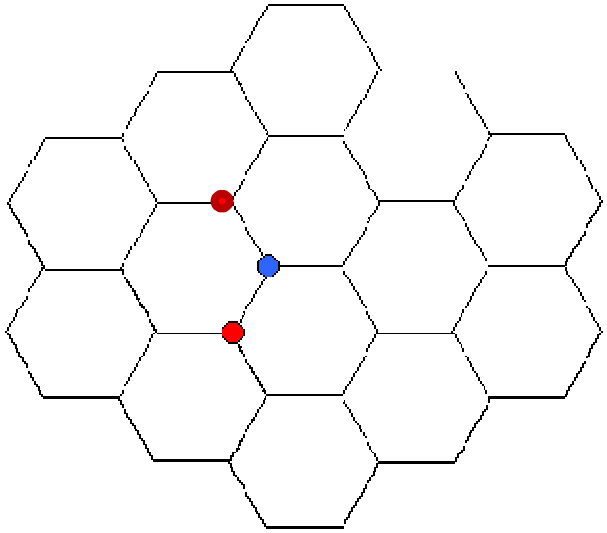


Nb film

2) Non-Bravais Lattice

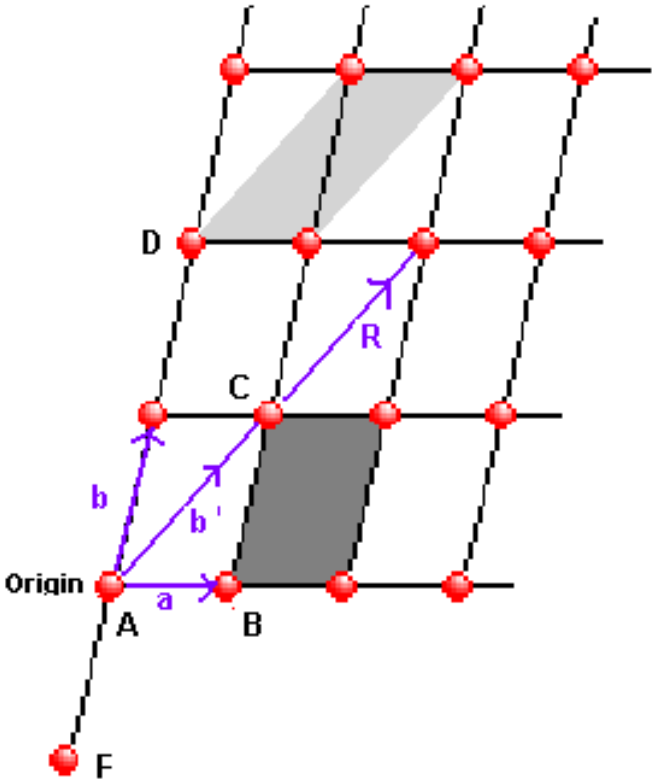
Not only the arrangement but also the orientation must appear exactly the same from every point in a bravais lattice.

- **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)

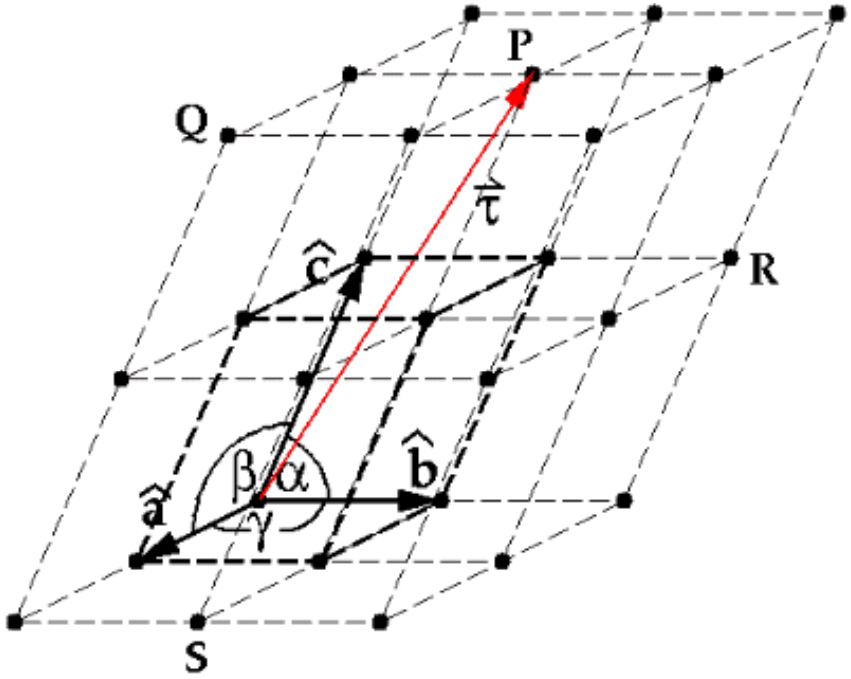
A space lattice is a set of points such that a translation from any point in the lattice by a vector;

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

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.

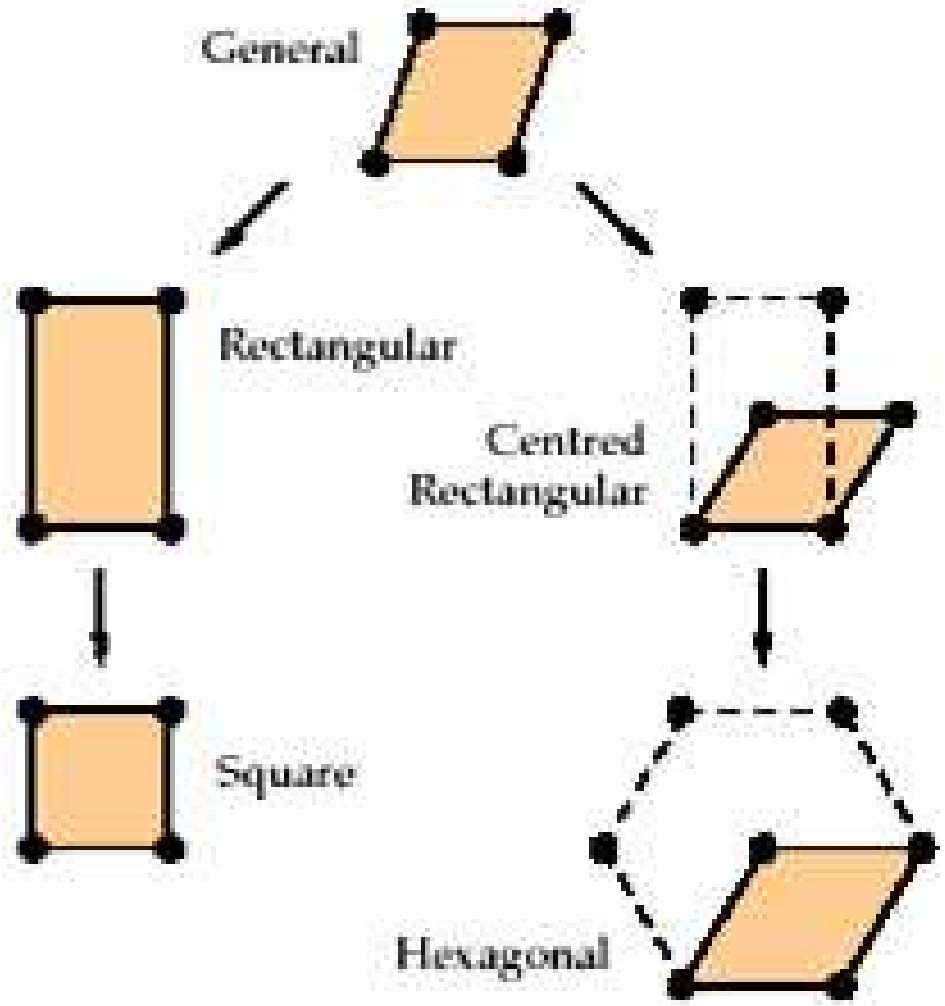
Lattice Vectors – 3D

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 n_1, n_2 and n_3 are arbitrary integers.



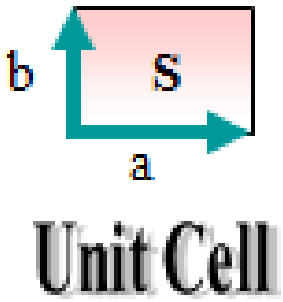
$$r = n_1 a + n_2 b + n_3 c$$

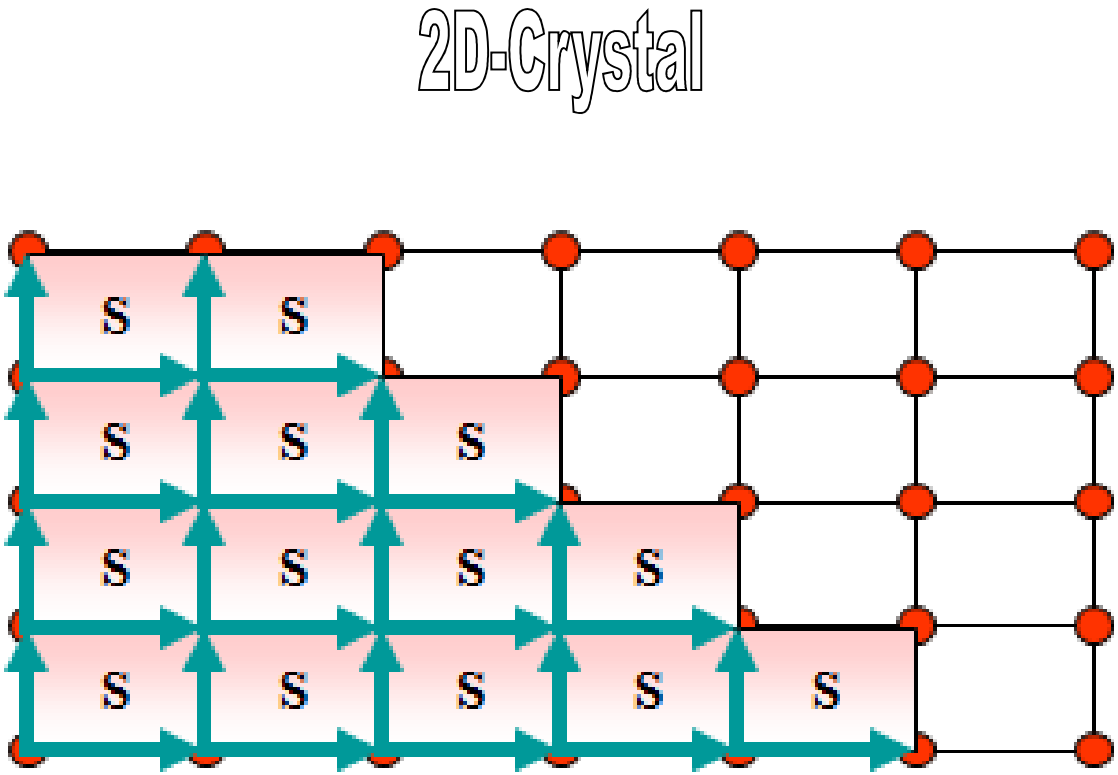
Five Bravais Lattices in 2D



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.



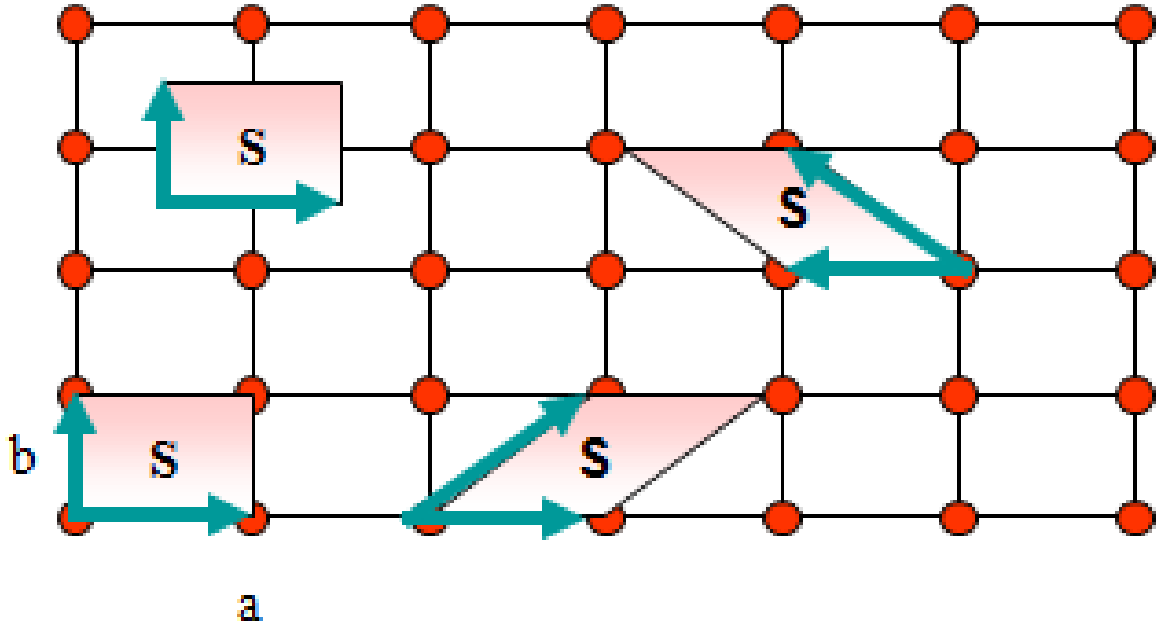


Unit Cell in 2D

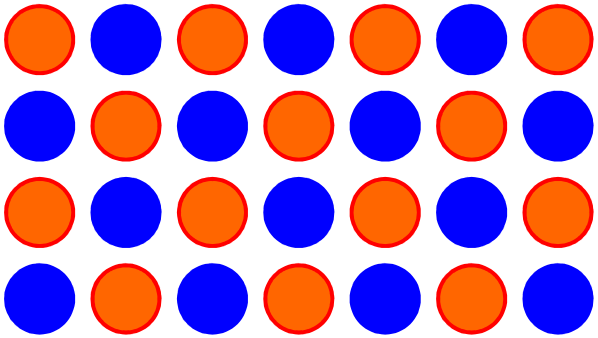
- **The smallest component of the crystal (group of atoms, ions or molecules), which when stacked together with pure translational repetition reproduces the whole crystal.**

2D-Crystal

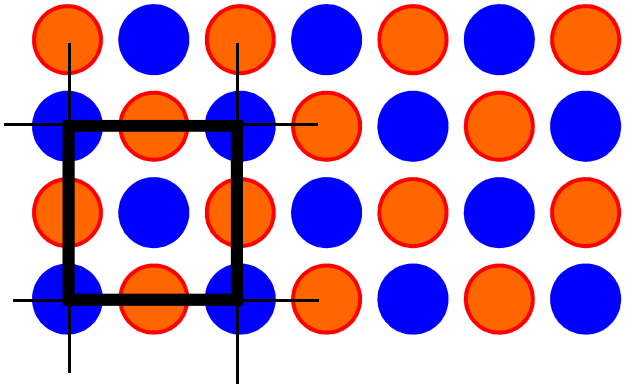
The choice of unit cell is not unique.



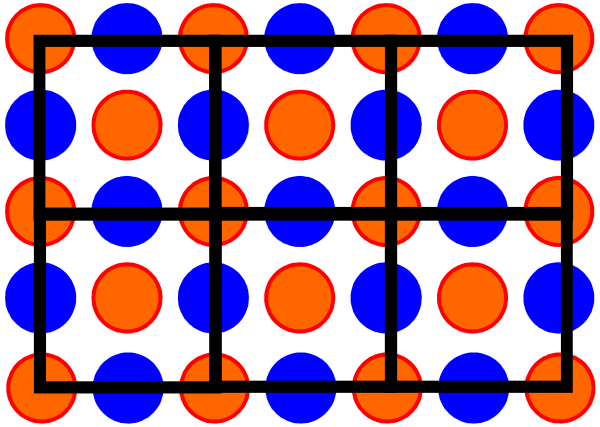
2D Unit Cell example -(NaCl)



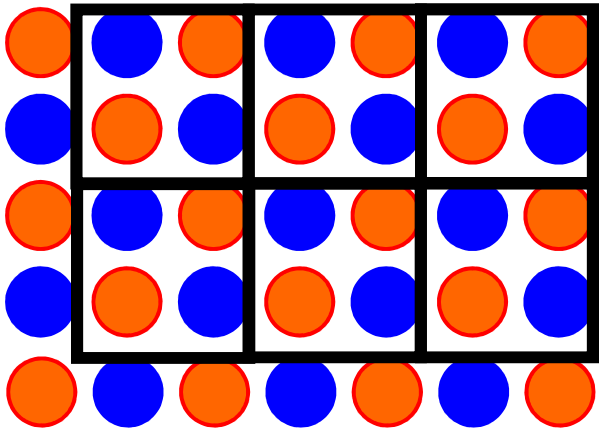
We define lattice points **; these are points with *identical environments***



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

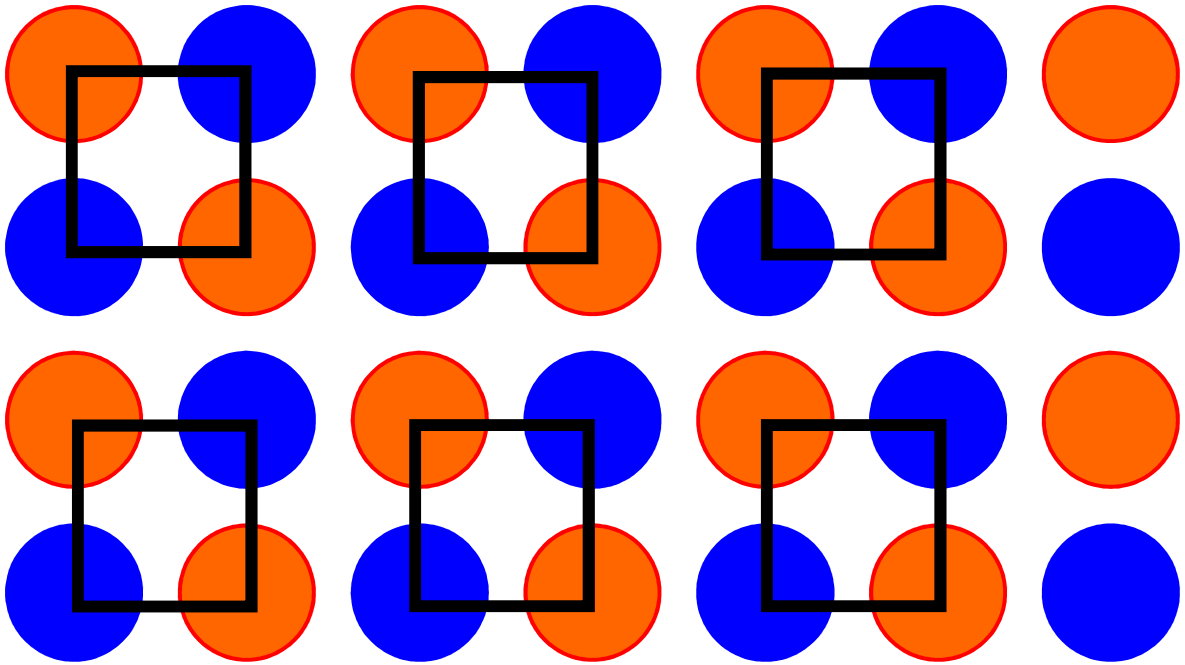


This is also a unit cell- it doesn't matter if you start from Na or Cl

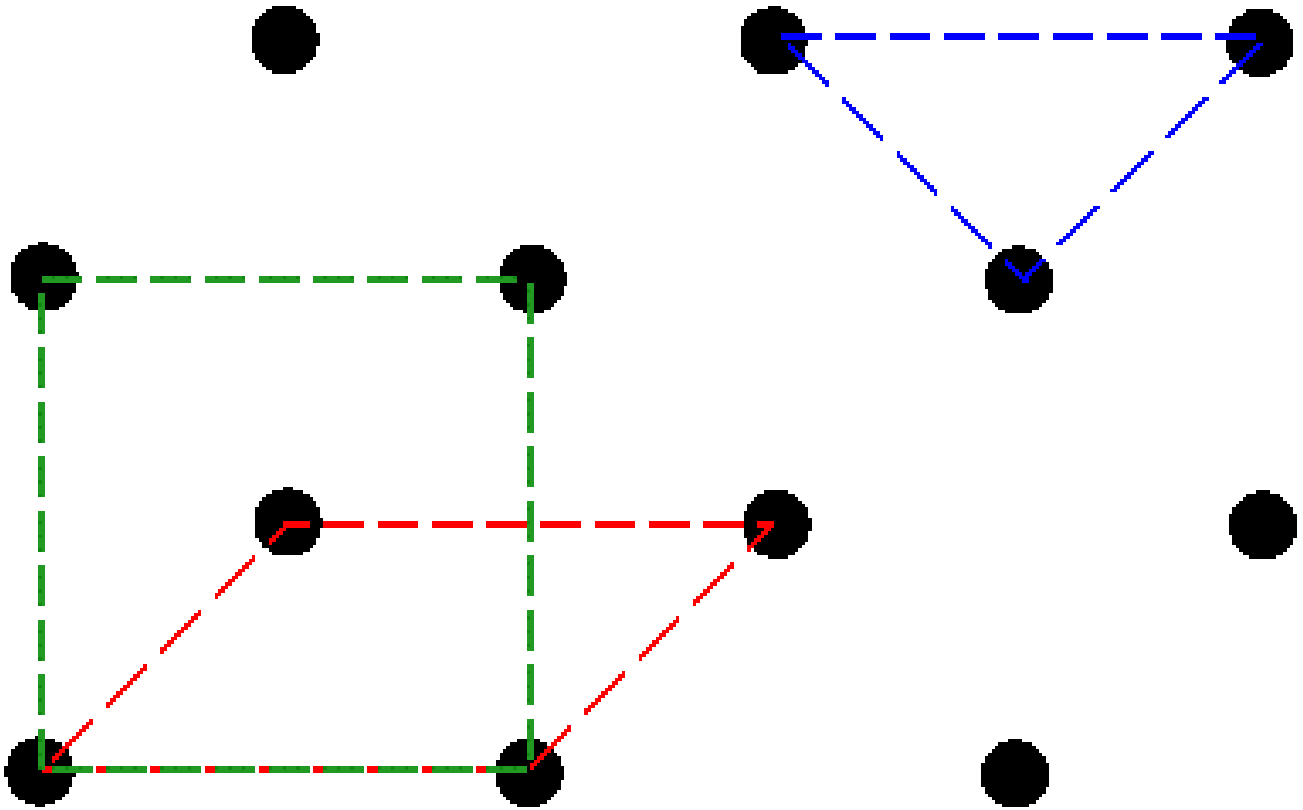


- or if you don't start from an atom

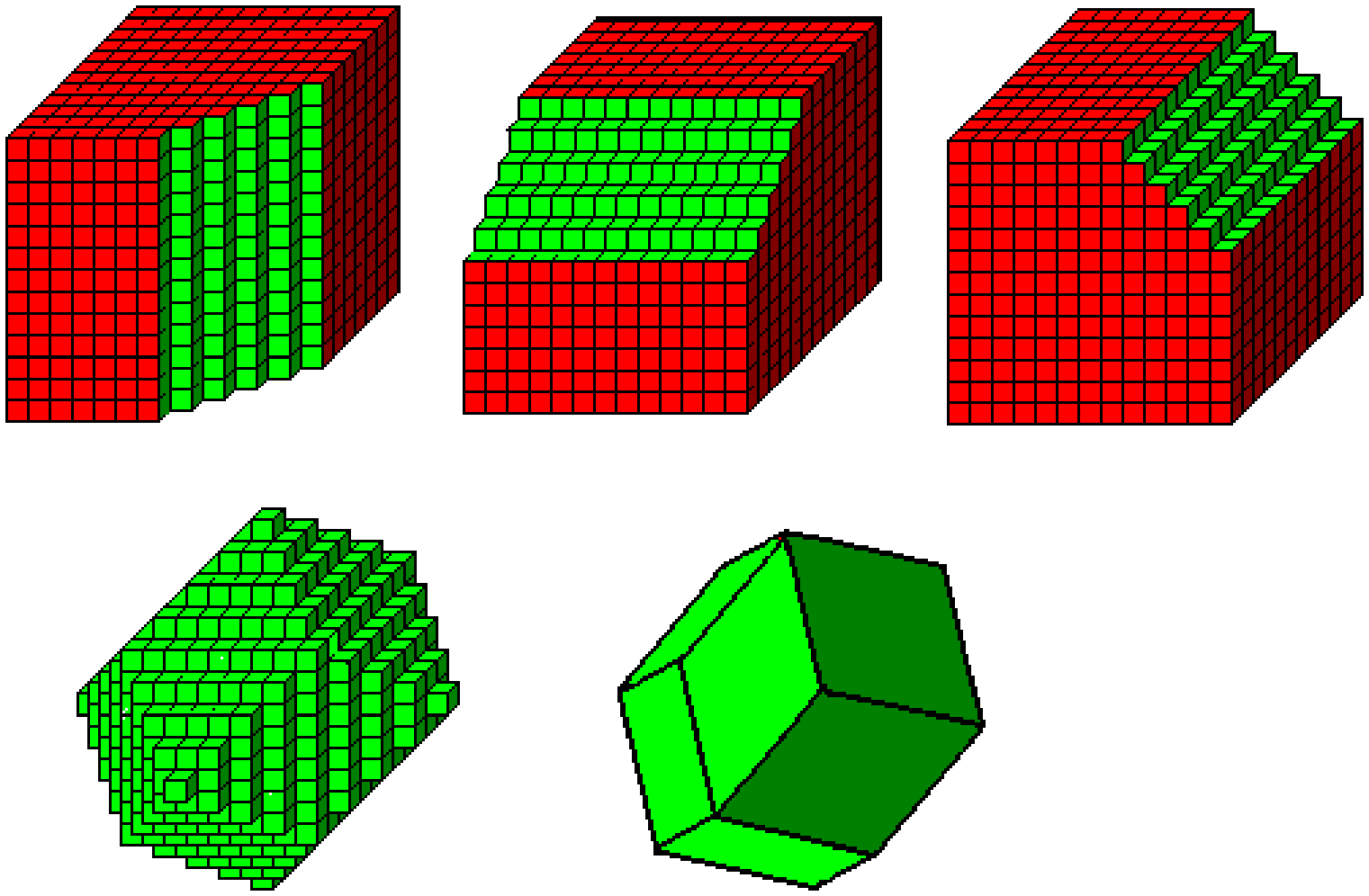
This is NOT a unit cell even though they are all the same - empty space is not allowed!

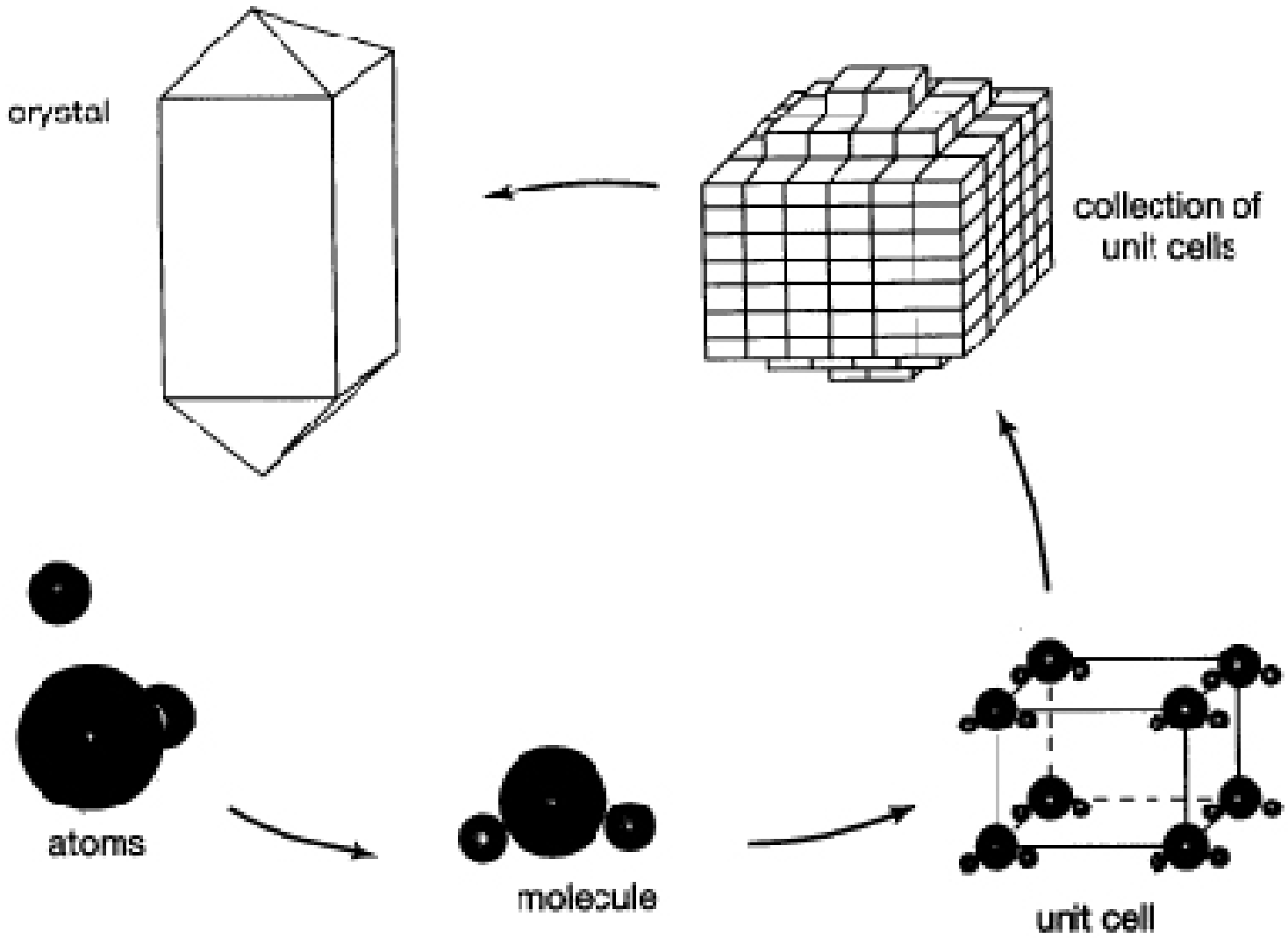


Why can't the blue triangle be a unit cell?

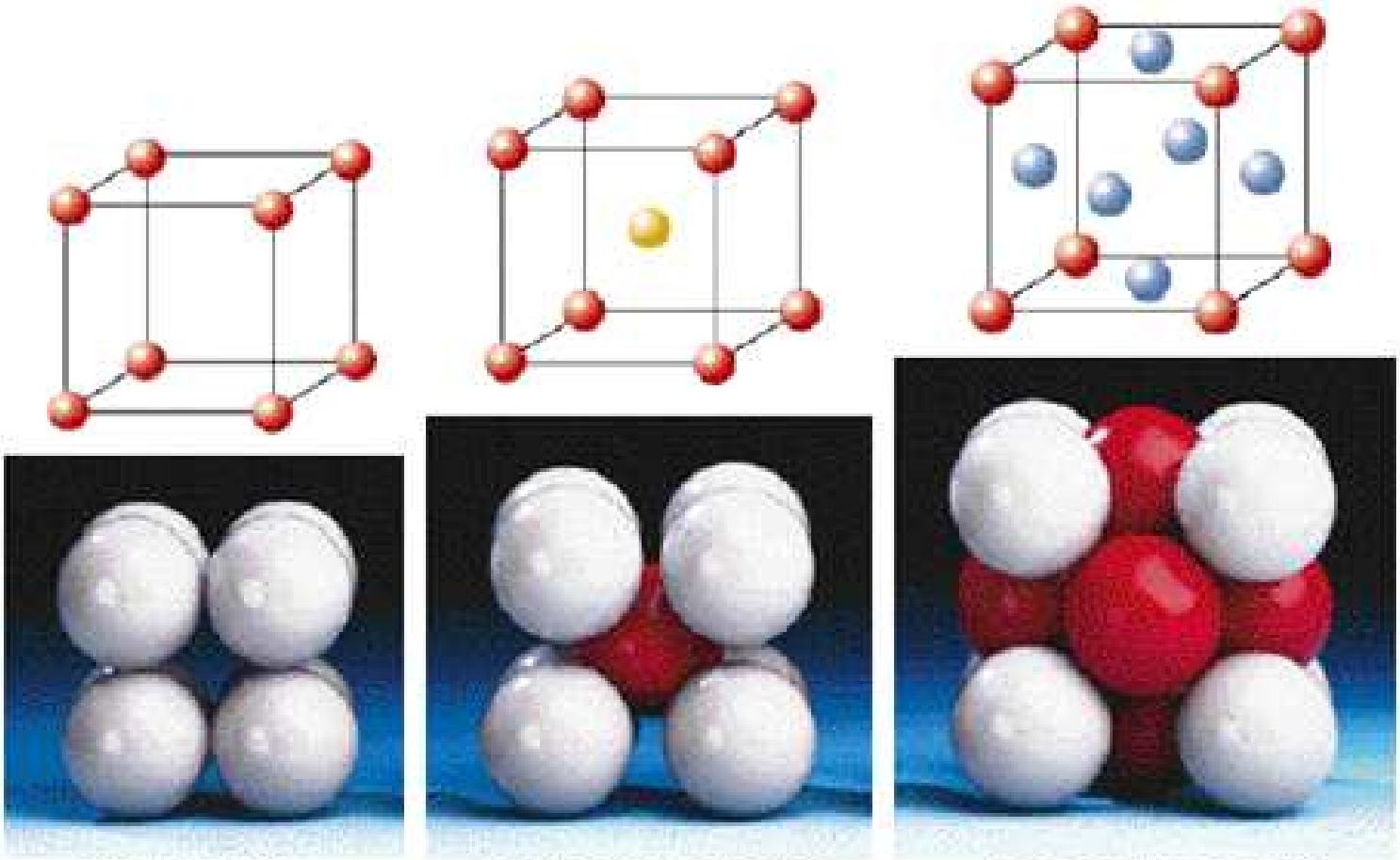


Unit Cell in 3D




crystal
collection of
unit cells
atoms
molecule
unit cell

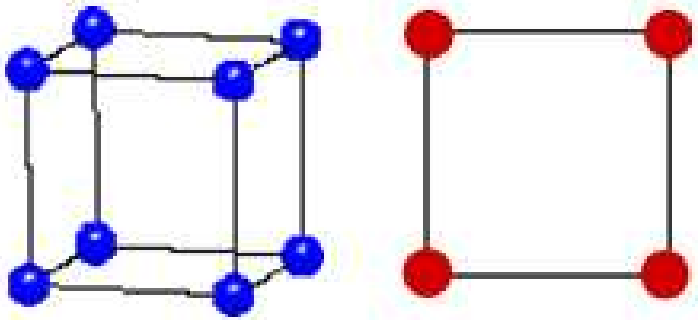
Three common Unit Cell in 3D



UNIT CELL

Primitive

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

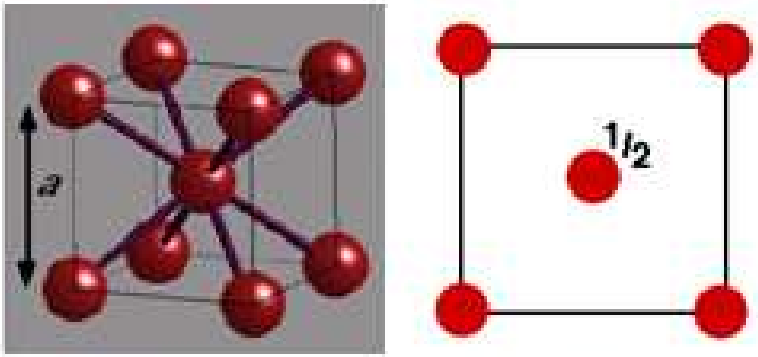


Simple cubic(sc)

Conventional = Primitive cell

Conventional & Non-primitive

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



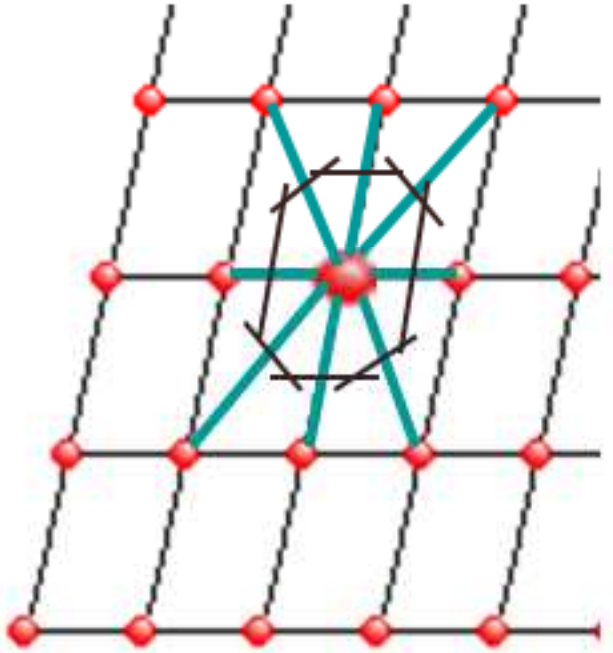
Body centered cubic(bcc)

Conventional ≠ Primitive cell

Wigner-Seitz Method

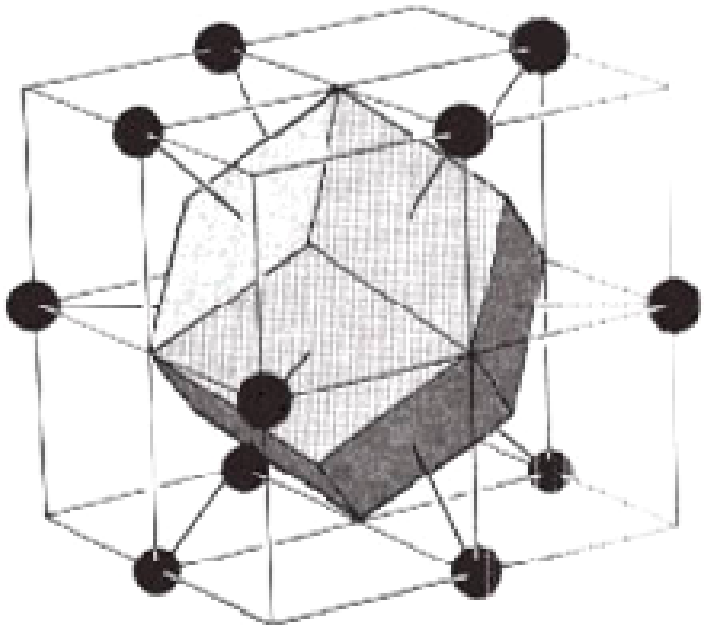
A simply way to find the primitive cell which is called Wigner-Seitz cell can be done as follows;

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.**

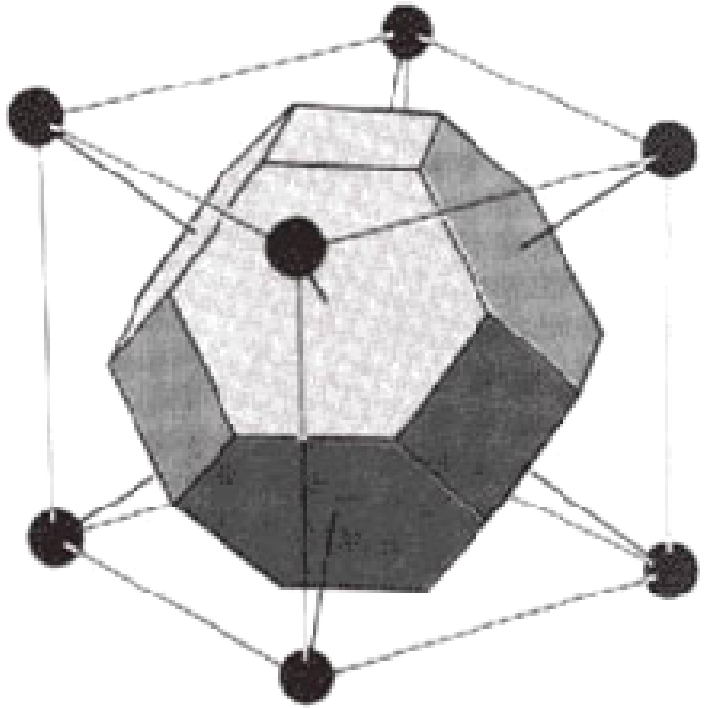


The volume enclosed is called as a Wigner-Seitz cell.

Wigner-Seitz cell in 3D

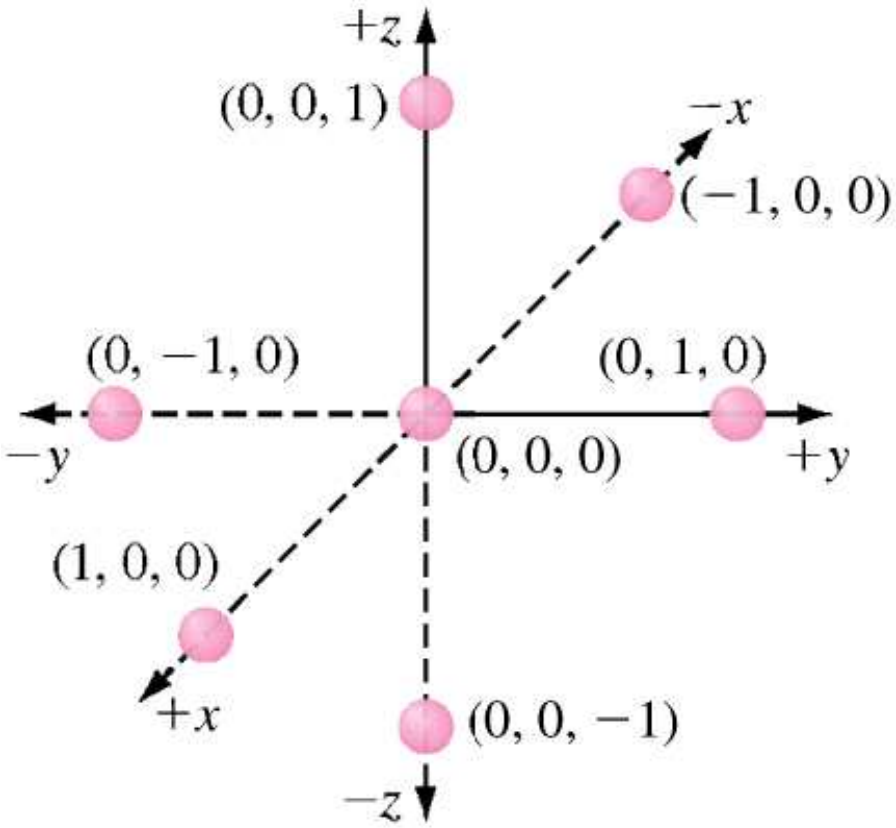


f.c.c Wigner-Seitz cell

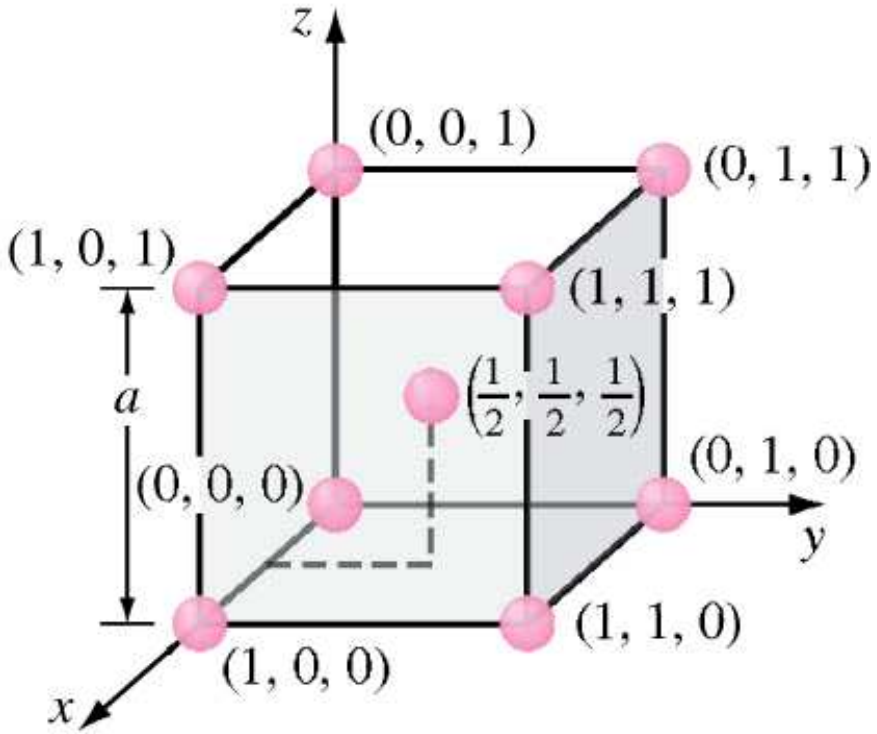


b.c.c Wigner-Seitz cell

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*.

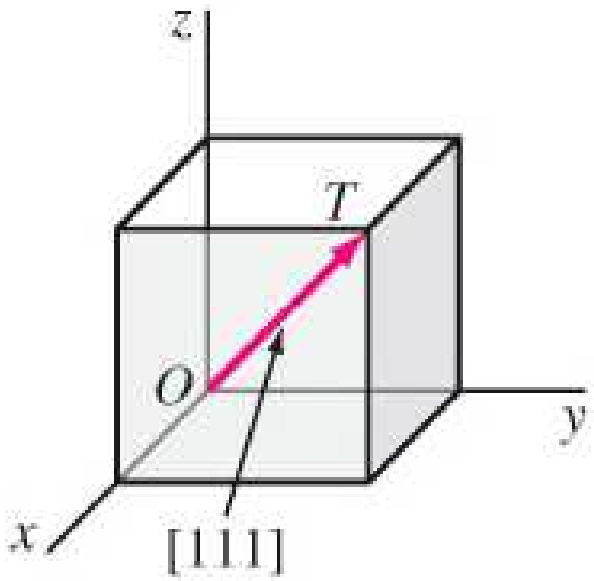
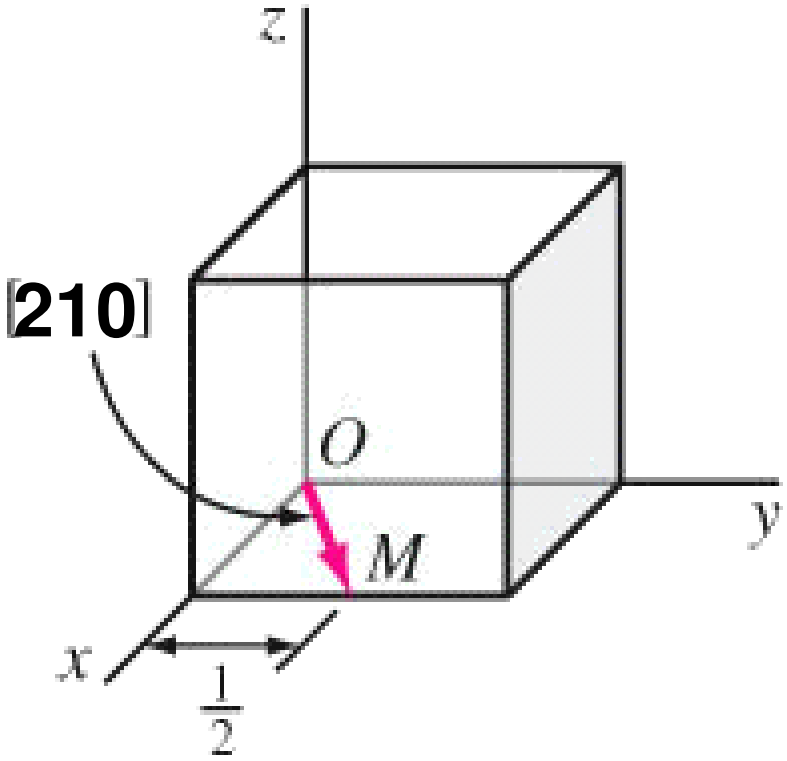
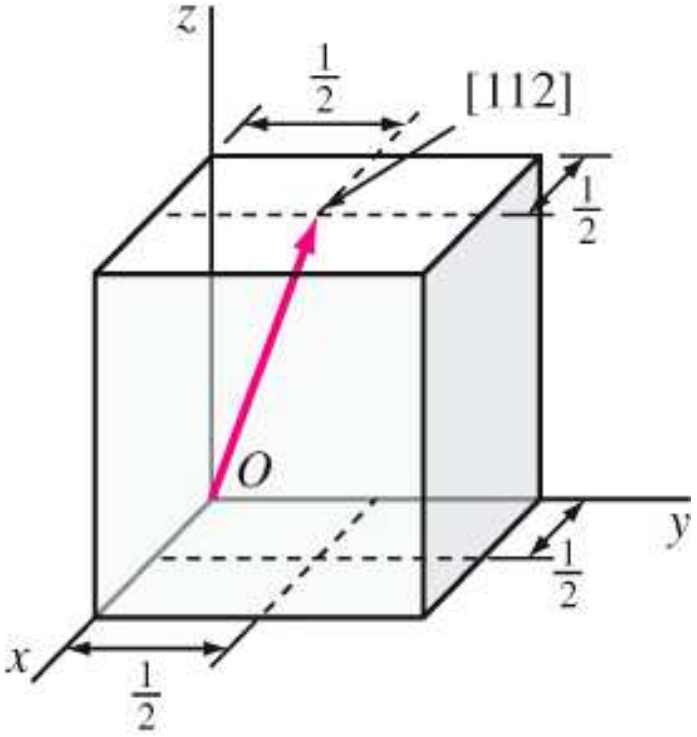


Fig. Shows [111] direction

Examples





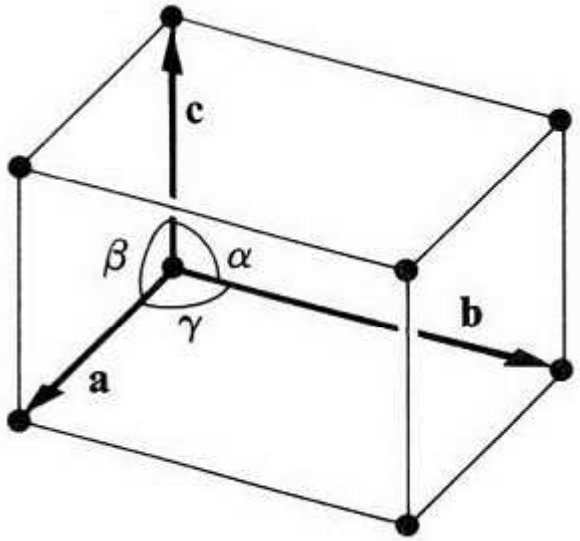
X = 1 , Y = ½ , Z = 0

[1 ½ 0] ⇨ [2 1 0]

X = ½ , Y = ½ , Z = 1

[½ ½ 1] [1 1 2]

Fourteen Bravais lattice and Seven Crystal Systems

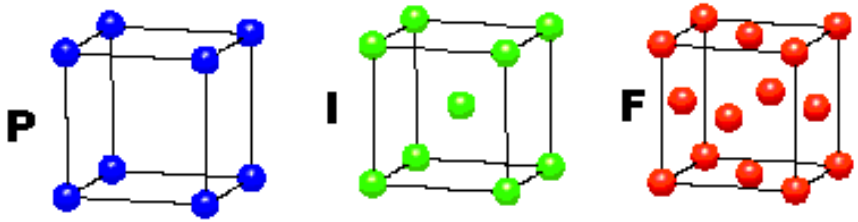


The Unit Cell is specified by the lengths of three basis vectors a, b, c. Also by the angles between these vectors

CUBIC

$a = b = c$

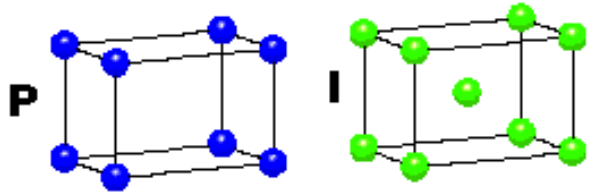
$\alpha = \beta = \gamma = 90°$



TETRAGONAL

$a = b \neq c$

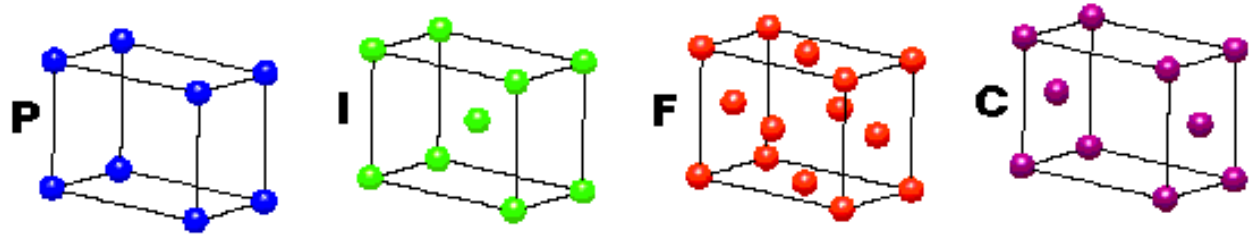
$\alpha = \beta = \gamma = 90°$



ORTHORHOMBIC

$a \neq b \neq c$

$\alpha = \beta = \gamma = 90°$

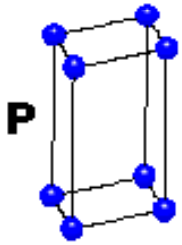


HEXAGONAL

$a = b \neq c$

$\alpha = \beta = 90°$

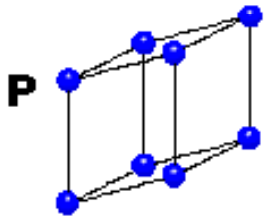
$\gamma = 120°$



TRIGONAL

$a = b = c$

$\alpha = \beta = \gamma \neq 90°$

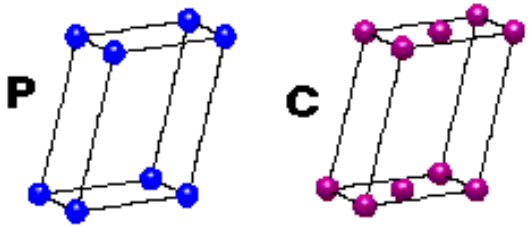


MONOCLINIC

$a \neq b \neq c$

$\alpha = \gamma = 90°$

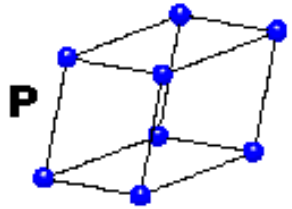
$\beta \neq 120°$



TRICLINIC

$a \neq b \neq c$

$\alpha \neq \beta \neq \gamma \neq 90°$



4 Types of Unit Cell
P = Primitive
I = Body-Centred
F = Face-Centred
C = Side-Centred
+
7 Crystal Classes
→ 14 Bravais Lattices

Table 1.1

The Seven Crystal Systems Divided into Fourteen Bravais Lattices

System	Bravais lattice	Unit cell characteristics	Characteristic symmetry elements
Triclinic	Simple	$a \neq b \neq c$ $\alpha \neq \beta \neq \gamma \neq 90^\circ$	None
Monoclinic	Simple Base-centered	$a \neq b \neq c$ $\alpha = \beta = 90^\circ \neq \gamma$	One 2-fold rotation axis
Orthorhombic	Simple Base-centered Body-centered Face-centered	$a \neq b \neq c$ $\alpha = \beta = \gamma = 90^\circ$	Three mutually orthogonal 2-fold rotation axes
Tetragonal	Simple Body-centered	$a = b \neq c$ $\alpha = \beta = \gamma = 90^\circ$	One 4-fold rotation axis
Cubic	Simple Body-centered Face-centered	$a = b = c$ $\alpha = \beta = \gamma = 90^\circ$	Four 3-fold rotation axes (along cube diagonal)
Trigonal (rhombohedral)	Simple	$a = b = c$ $\alpha = \beta = \gamma \neq 90^\circ$	One 3-fold rotation axis
Hexagonal	Simple	$a = b \neq c$ $\alpha = \beta = 90^\circ$ $\gamma = 120^\circ$	One 3-fold rotation axis

Some General Characteristics of Bravais lattices of Crystal Systems

- Simple lattice has only points at the corners
- A body centered has an additional point at the center of cell.
- A face centered has six additional points, one on each face.

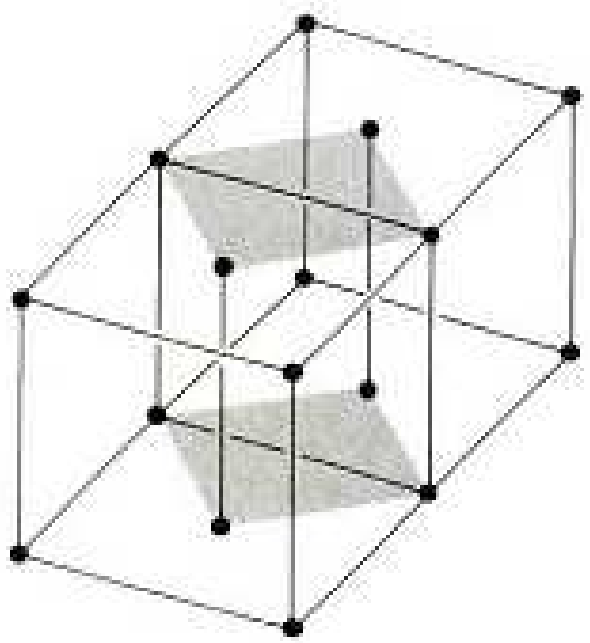
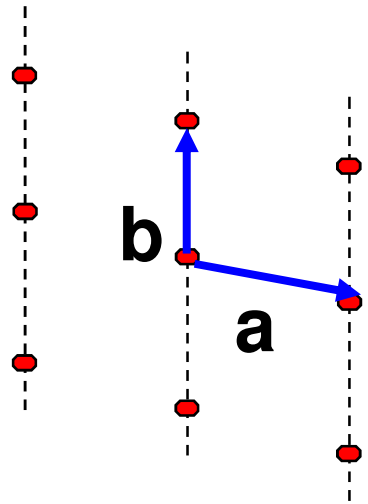


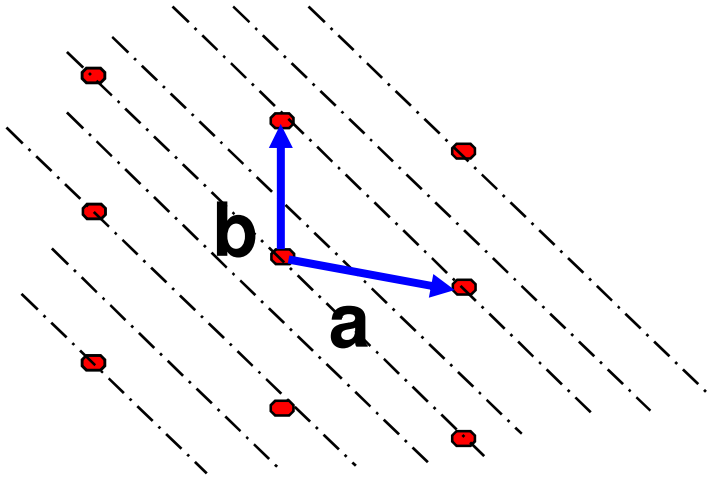
Fig. 1.8 A base-centered tetragonal is identical to a simple tetragonal of a different unit cell. Shaded areas are the basis of the simple tetragonal cell.

Crystal Planes

- **Within a crystal lattice it is possible to identify sets of equally spaced parallel planes. These are called lattice planes.**
- **In the figure density of lattice points on each plane of a set is the same and all lattice points are contained on each set of planes.**

The set of planes in 2D lattice.





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.

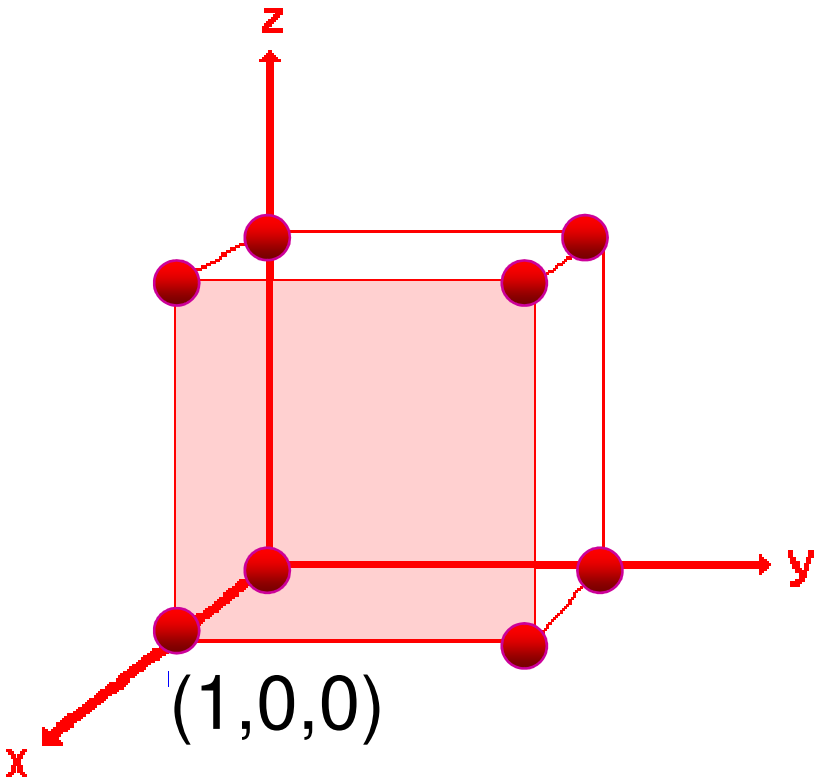
To determine Miller indices of a plane, take the following steps;

1) Determine the intercepts of the plane along each of the three crystallographic directions

2) Take the reciprocals of the intercepts

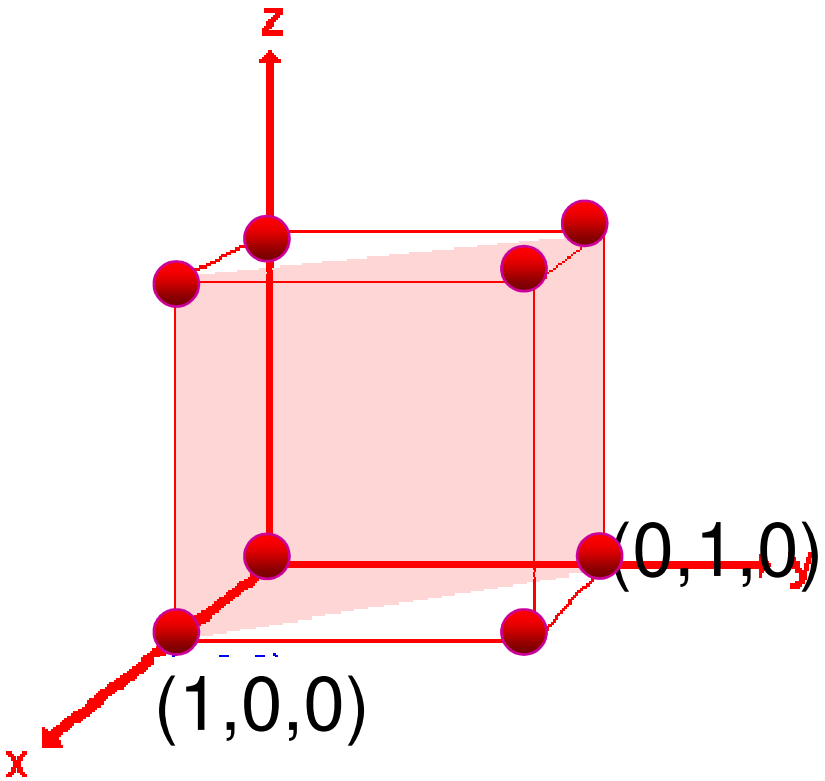
3) If fractions result, multiply each by the denominator of the smallest fraction

Example-1



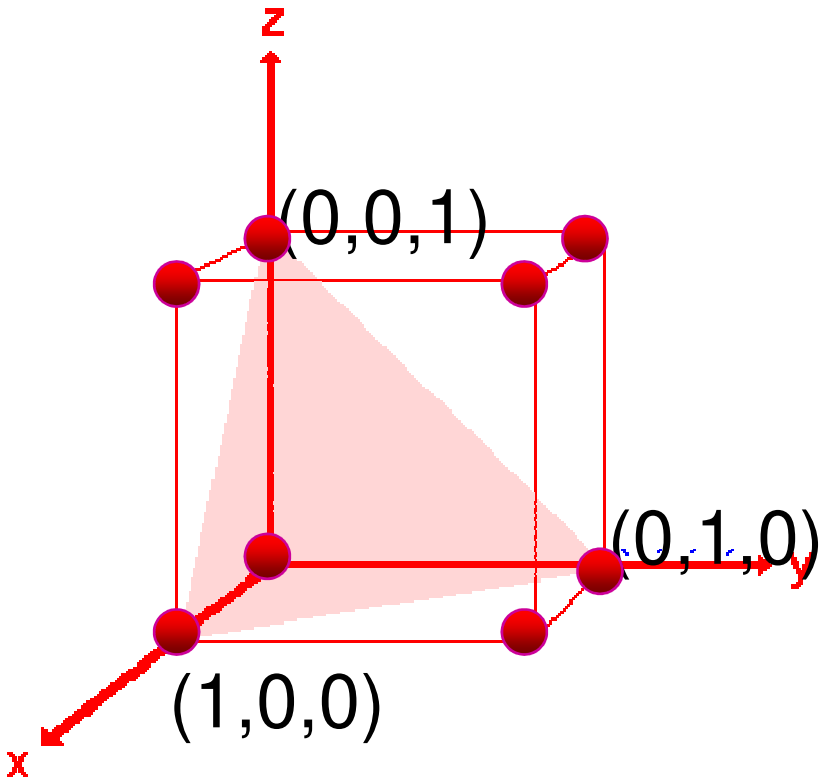
Axis	X	Y	Z
Intercept points	**1**	∞	∞
Reciprocals	**1/1**	**1/ ∞**	**1/ ∞**
Smallest Ratio	**1**	**0**	**0**
Miller İndices (100)			

Example-2



Axis	X	Y	Z
Intercept points	1	1	∞
Reciprocals	1/1	1/ 1	1/ ∞
Smallest Ratio	1	1	0
Miller İndices			**(110)**

Example-3



Axis	X	Y	Z
Intercept points	1	1	1
Reciprocals	1/1	1/ 1	1/ 1
Smallest Ratio	1	1	1
Miller İndices (111)			