Hexagonal close packed structure

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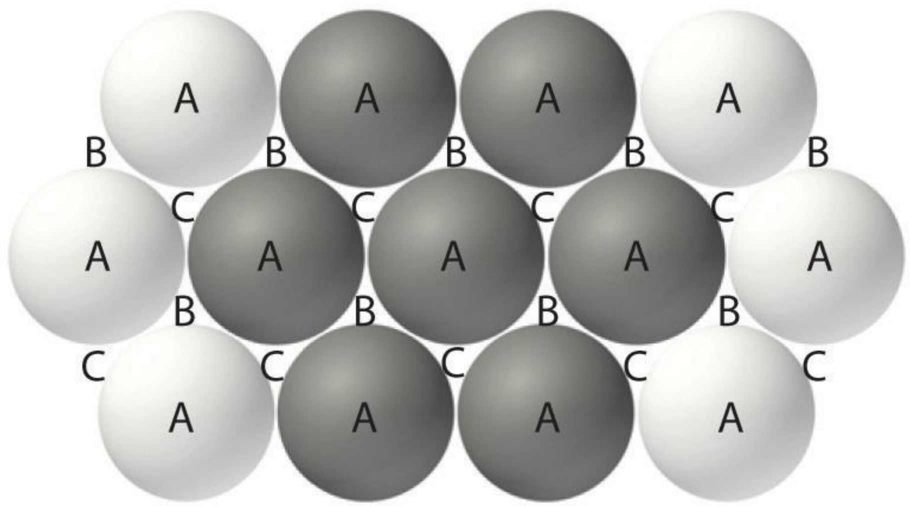
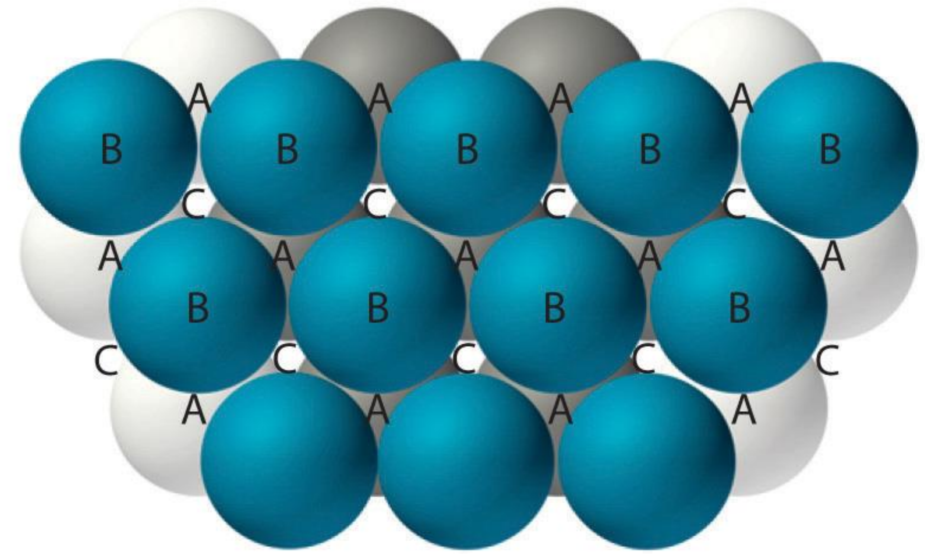
Close packed structures

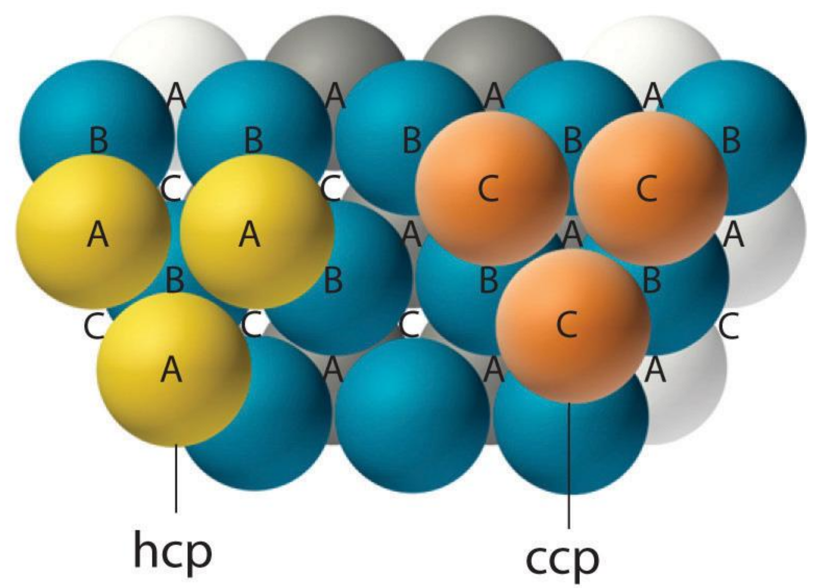
Close packed structures have highest density in a unit cell



(a) Single layer



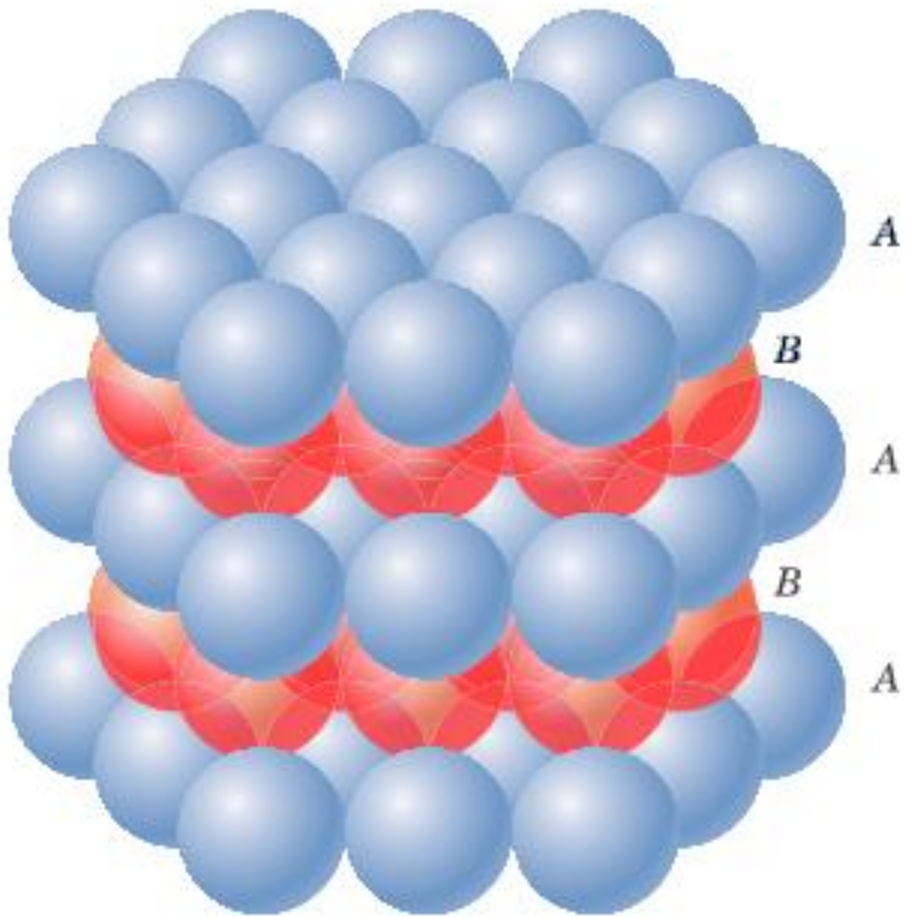
(b) Two layers

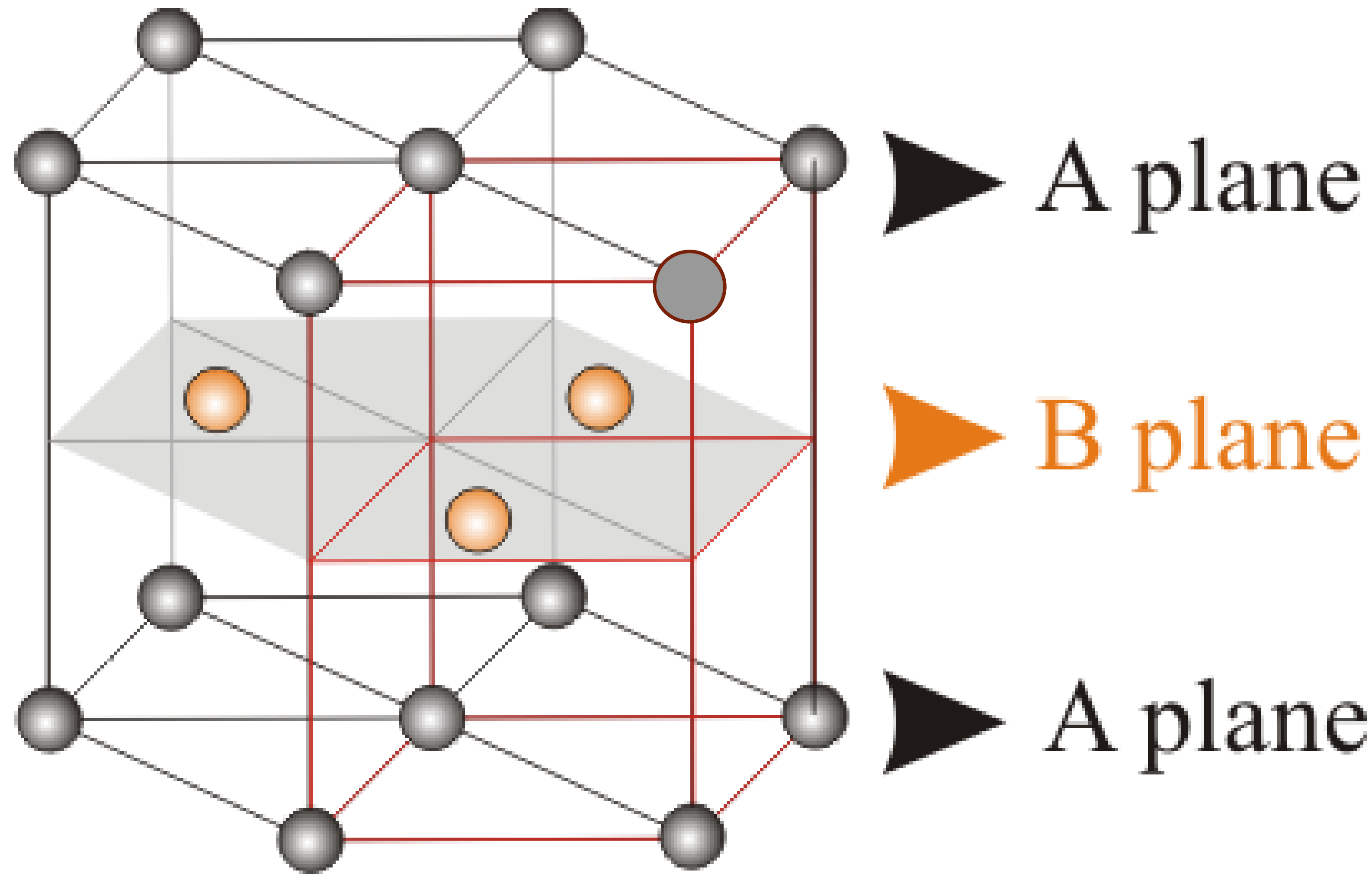


(c) Three layers

Hexagonal close packed cubic (HCP)

HCP is a close packed structures

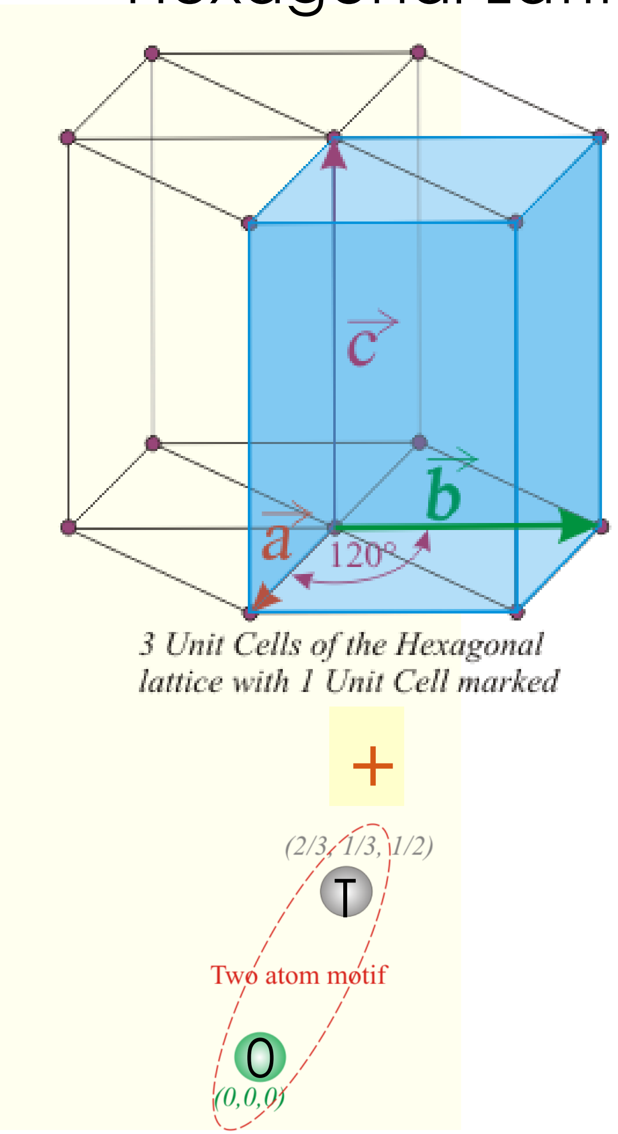




Showing 3 unit cells and the rhombic prism UC

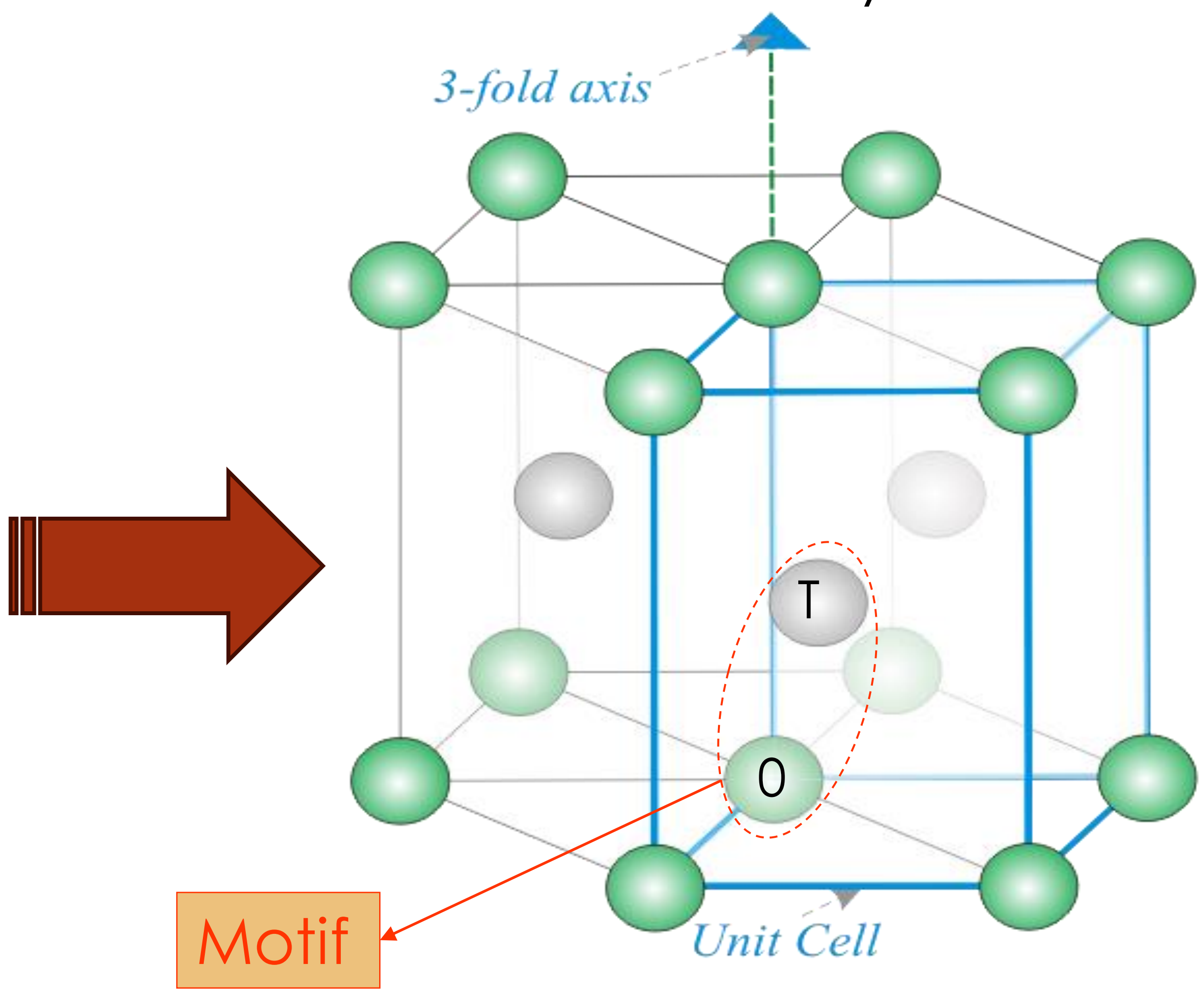
- LATTICE → Hexagonal **HCP**
- MOTIF → Atoms at: O(0,0,0) & T(⅔, ⅓,½)

Hexagonal Lattice



Two atom Motif

HCP crystal



Hexagonal close packed structure (HCP)

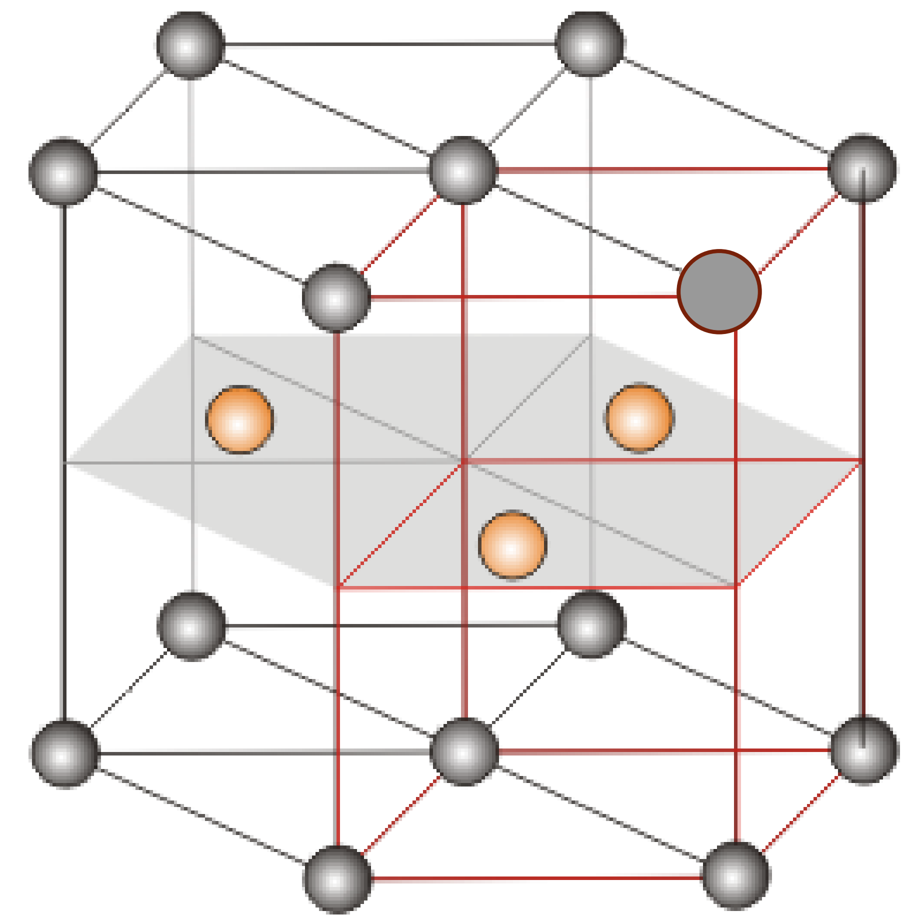
Lattice points in a unit cell: 6

No. of atoms in a unit cell: 6

Basis(No. of atoms/lattice point): 1

Co-ordination number: 12

Relation of a and r: a = 2r

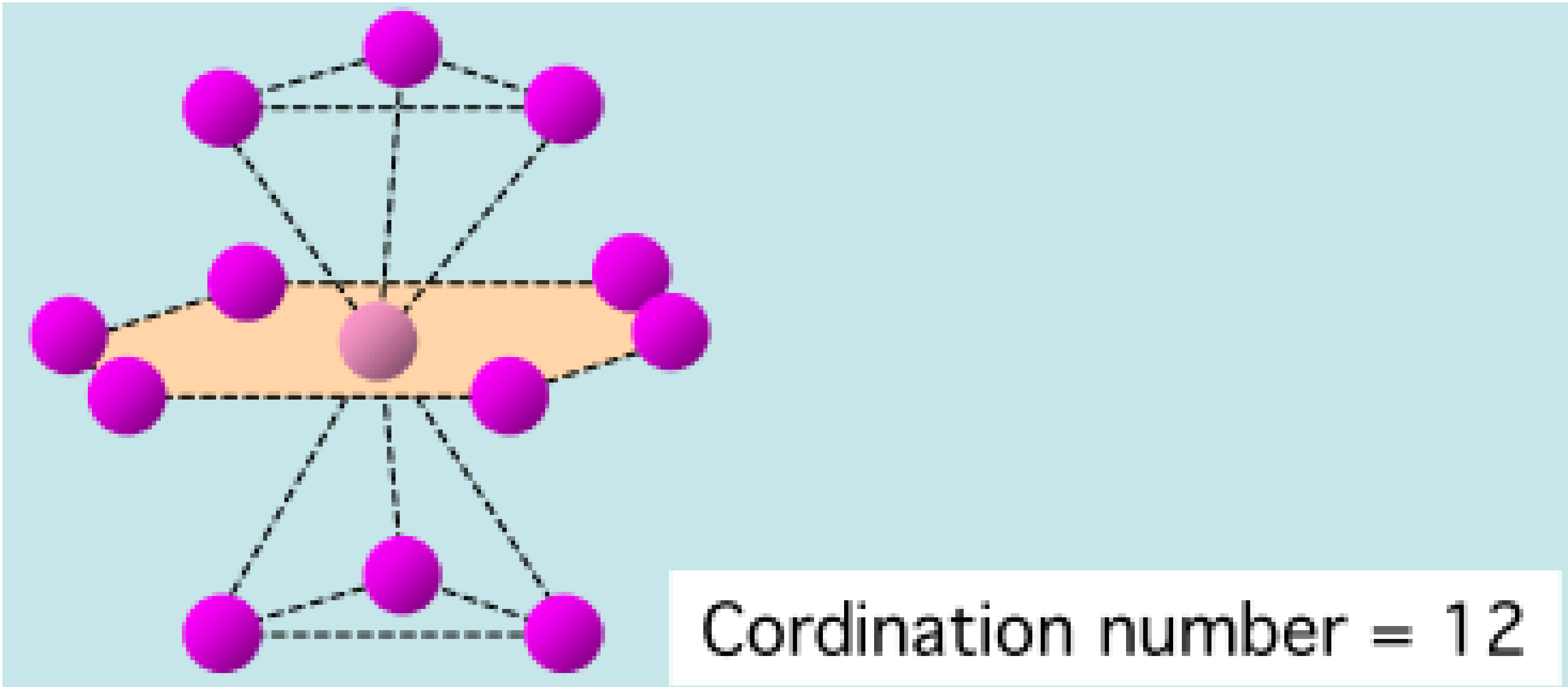


Examples

1) Cobalt
2) Cadmium
3) Zinc
4) α-titanium
5) Magnesium

Co-ordination number(CN)

No. of nearest neighbors (No. of atoms touching)



HCP

c/a Ratio and APF in HCP

Derivations are uploaded on LMS

$$\frac{c}{a} = \sqrt{\frac{8}{3}} = 1.663$$

APF = 74%

Planes in Hexagonal close-packed system

Miller-Bravais index notations for planes

- Directions and planes in hexagonal lattices and crystals are designated by the 4-index Miller-Bravais notation.
- In the four-indexed notation:
  - The first three indices are a symmetrically related set on the basal plane.
  - The third index is a *redundant one* and is introduced to make sure that members of a family of directions or planes have a set of identical numbers
  - The fourth index represents the 'c' axis *(⊥ to the basal plane)*.

Miller-Bravais index notations for planes

- The redundant index can be obtained from the other two.
- This is called a symmetry condition. If this condition gets satisfied, then and only then the plane exists.

$$(h\ k\ i\ l)$$

$$h + k + i = 0$$

or

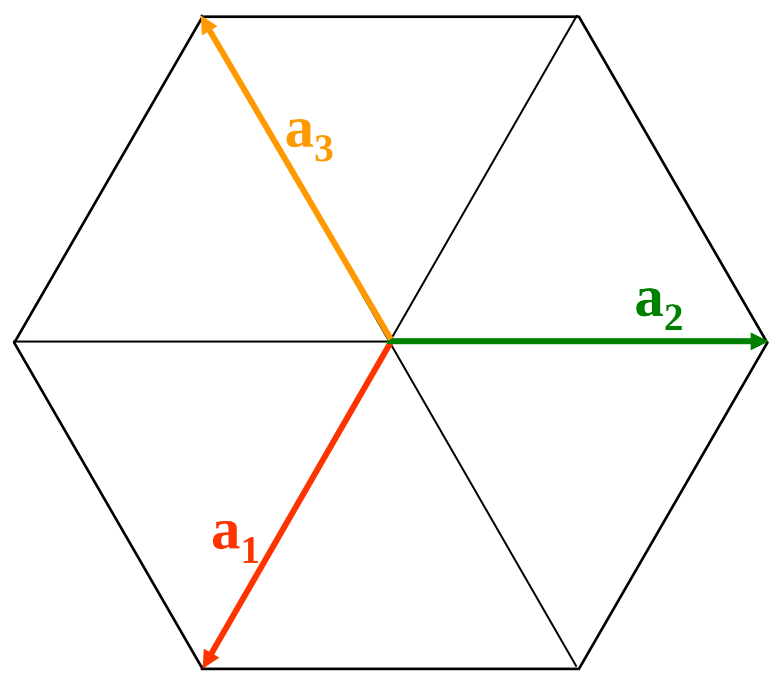
$$i = -(h + k)$$

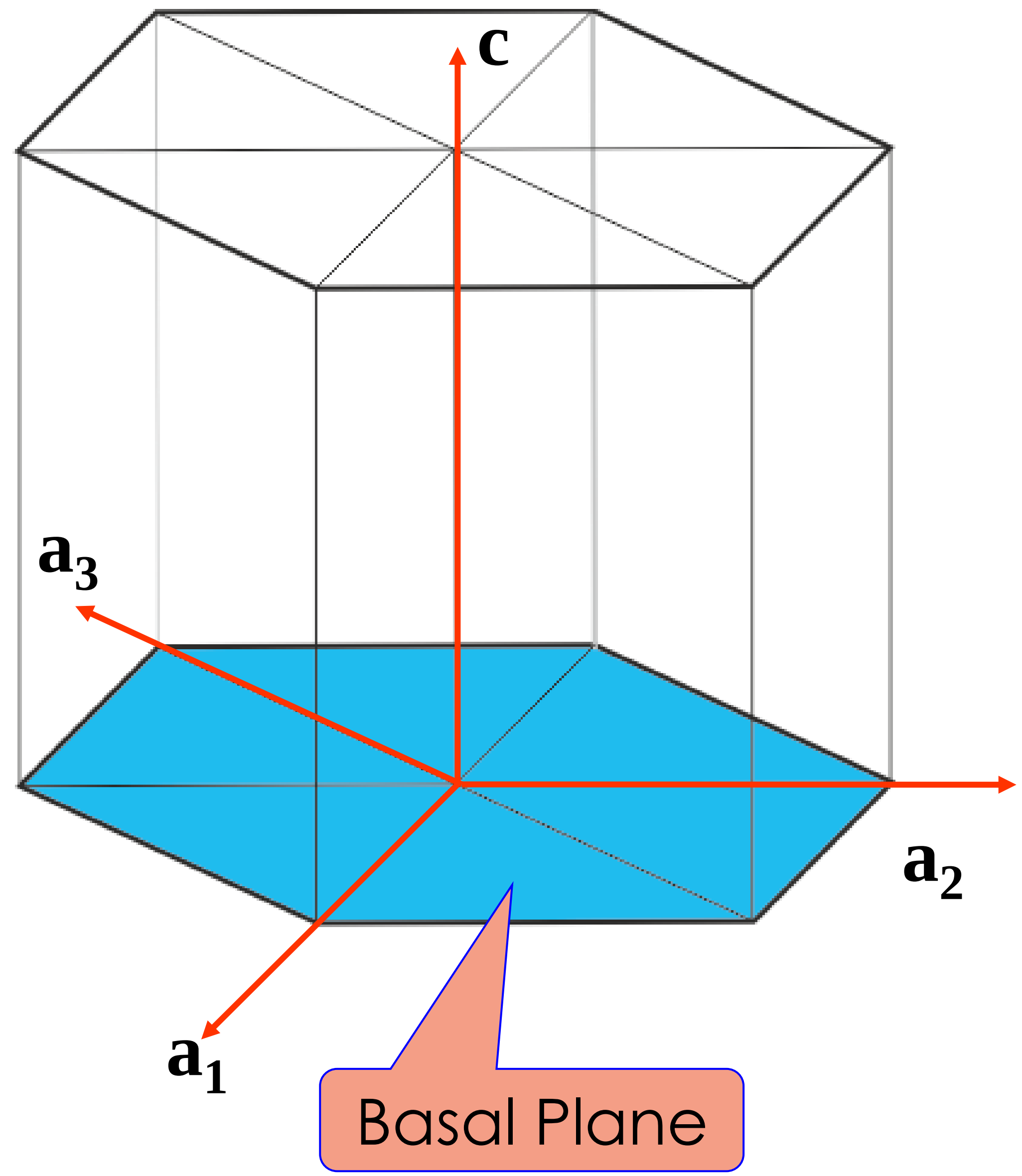
$$(hkl) \rightarrow (hkil)$$

$$(110) \rightarrow (11\bar{2}0)$$

M-B Indices for planes in HCP

Basal Plane





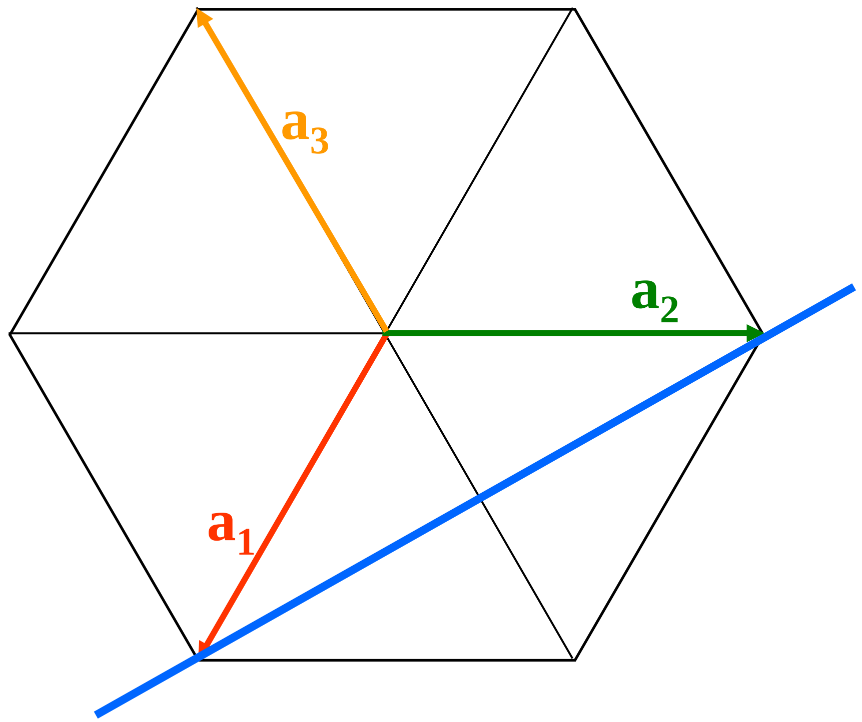
Intercepts $\rightarrow \infty\ \infty\ \infty\ \ 1$

Miller $\rightarrow (0\ 0\ 1)$

Miller-Bravais $\rightarrow (0\ 0\ 0\ 1)$

M-B Indices for planes in HCP

Prism planes

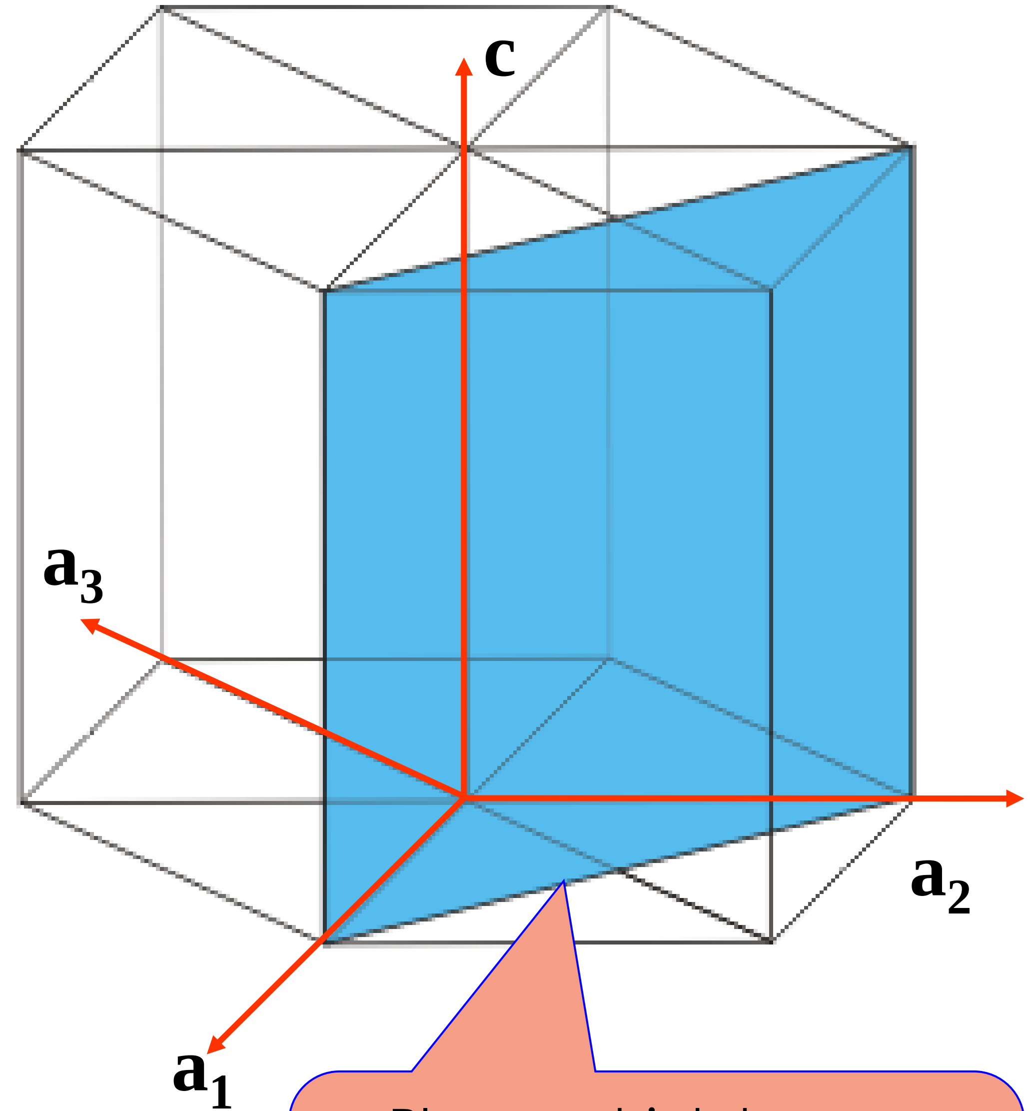


(h k i l)
i = –(h + k)

Intercepts → 1 1 - ½ ∞

Miller → (1 1 0)

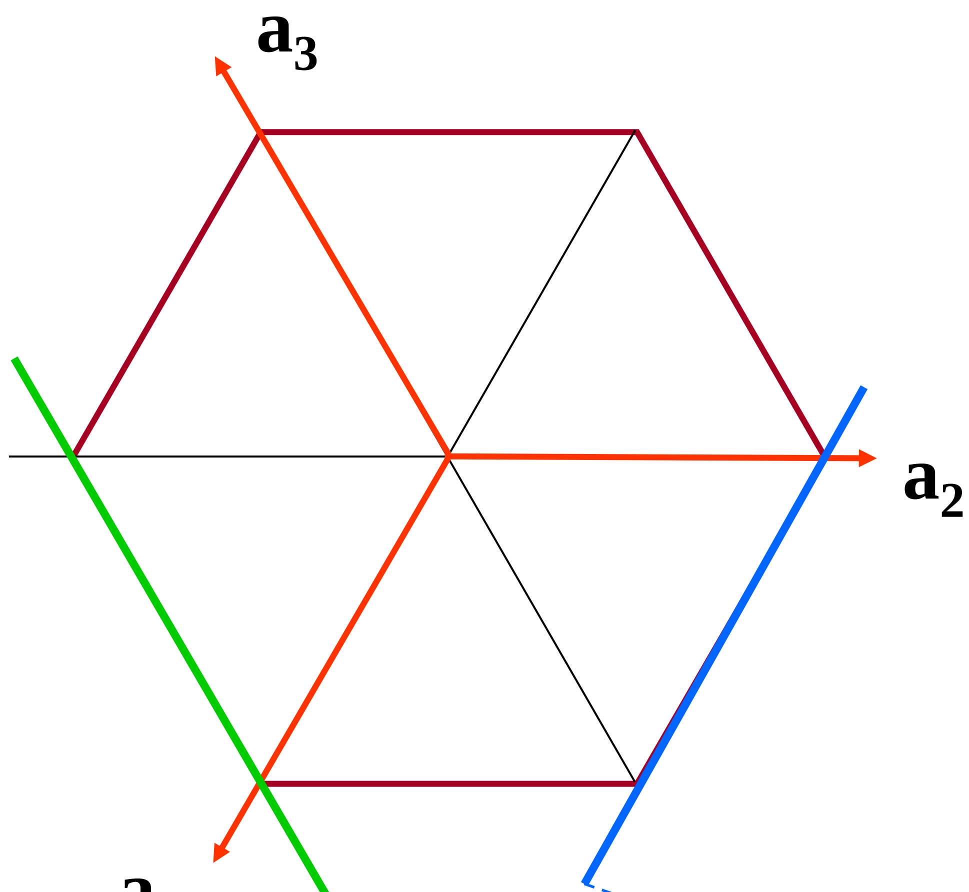
Plane → $(1\ 1\ \bar{2}\ 0)$

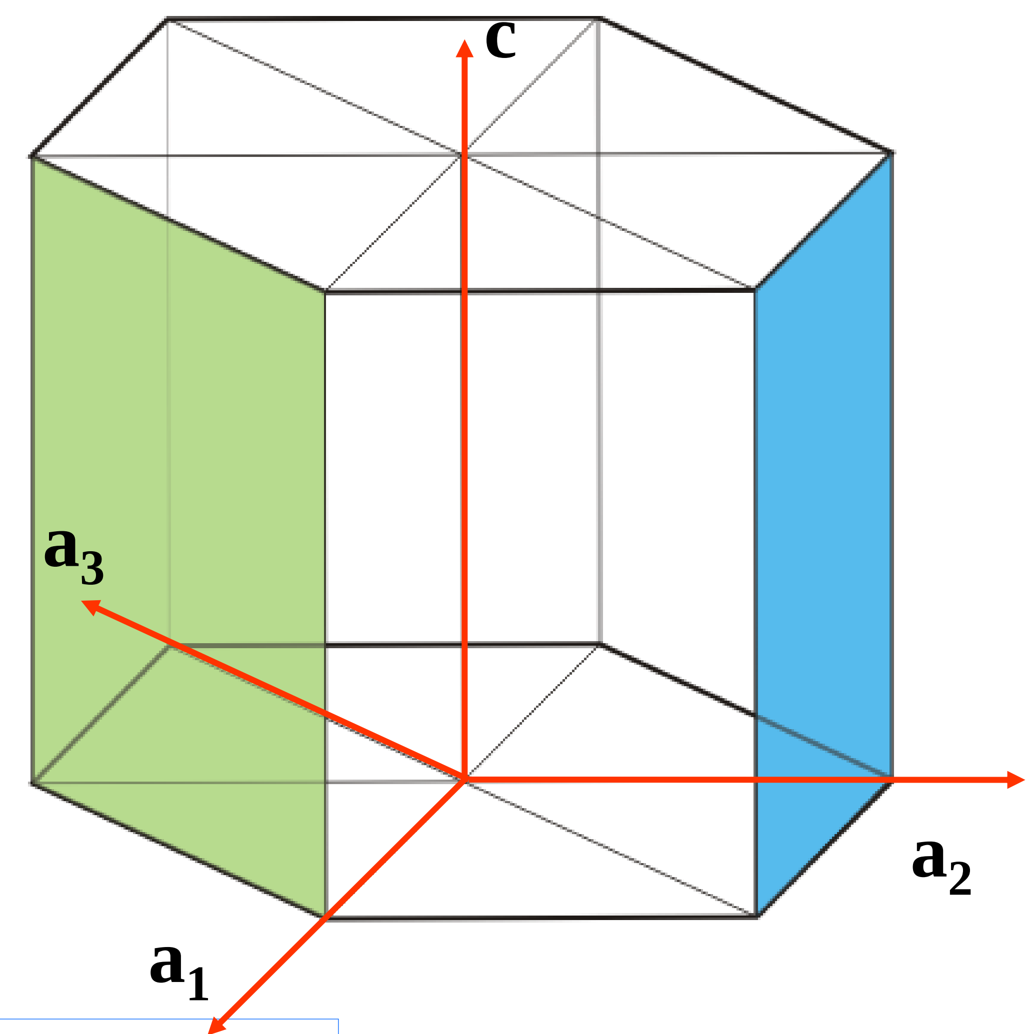


Planes which have ∞ intercept along c-axis (i.e., vertical planes) are called Prism planes

M-B Indices for planes in HCP

Green' and 'blue' planes belong to the same family





Intercepts → $1\ -1\ \infty\ \infty$

Miller → $(1\ \bar{1}\ 0)$

Miller-Bravais → $(1\ \bar{1}\ 0\ 0)$

Intercepts → $\infty\ 1\ -1\ \infty$

Miller → $(0\ 1\ 0)$

Miller-Bravais → $(0\ 1\ \bar{1}\ 0)$

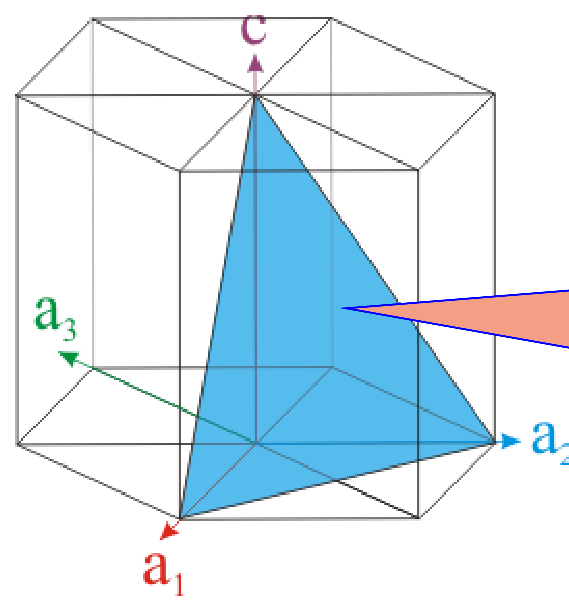
M-B Indices for planes in HCP

Pyramidal planes

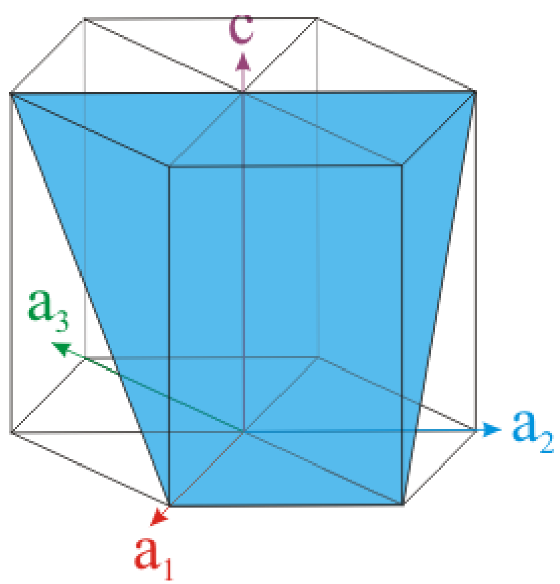
Intercepts $\rightarrow \infty\ 1\ -1\ \ \infty$

Miller $\rightarrow (0\ 1\ 0)$

Miller-Bravais $\rightarrow (0\ 1\ \ \bar{1}\ \ 0)$



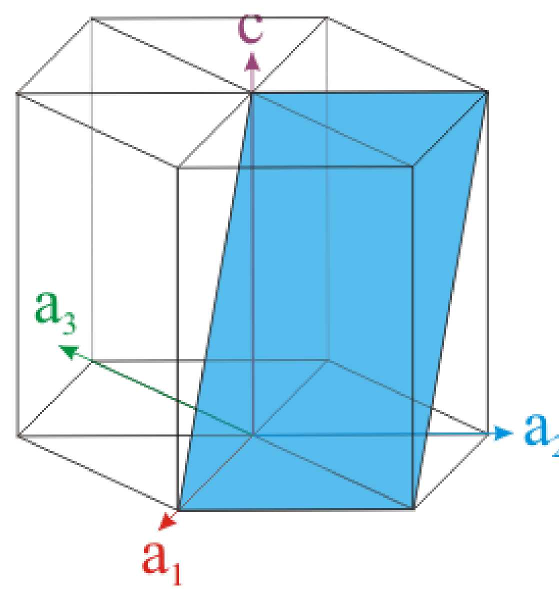
Inclined planes which have finite intercept along c-axis are called Pyramidal planes



Intercepts $\rightarrow \infty\ 1\ -1\ \ \infty$

Miller $\rightarrow (0\ 1\ 0)$

Miller-Bravais $\rightarrow (0\ 1\ \ \bar{1}\ \ 0)$

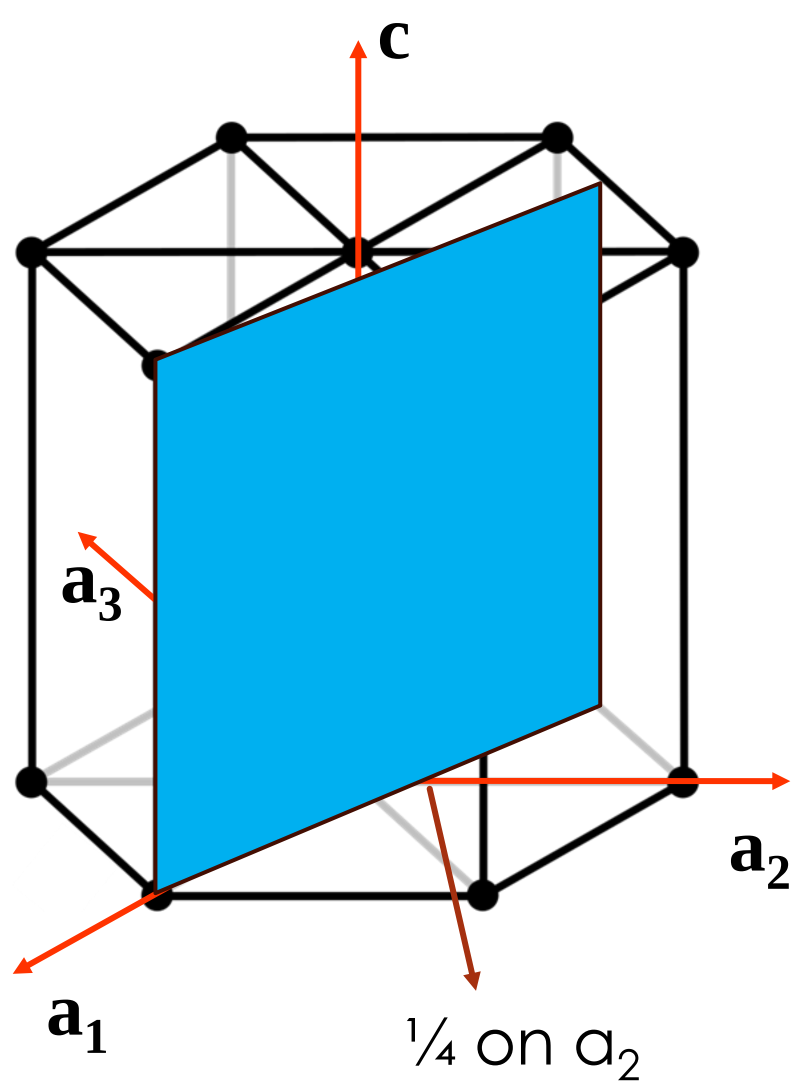


Intercepts $\rightarrow \infty\ 1\ -1\ \ \infty$

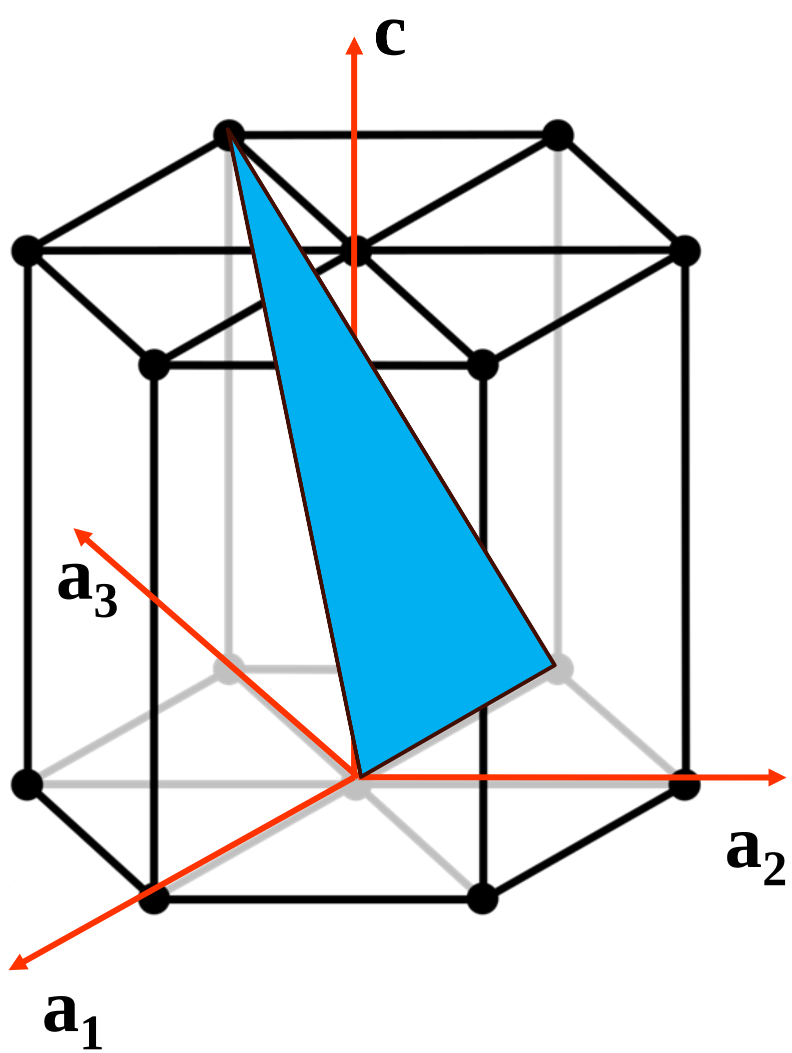
Miller $\rightarrow (0\ 1\ 0)$

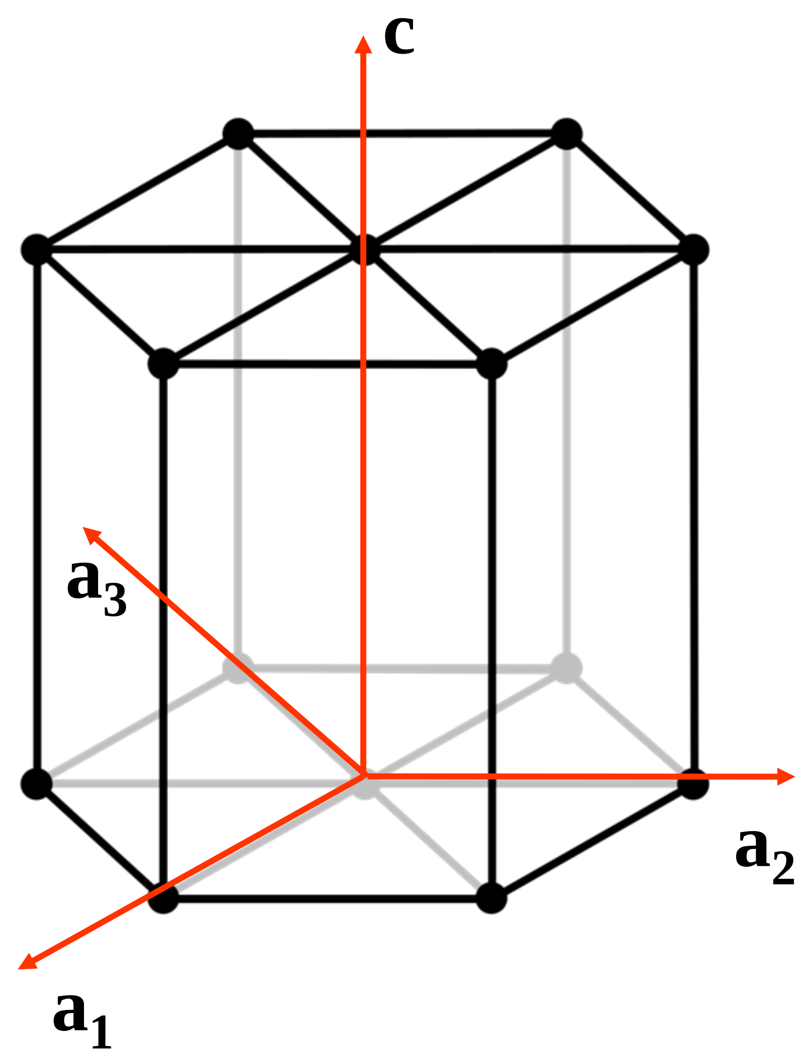
Miller-Bravais $\rightarrow (0\ 1\ \ \bar{1}\ \ 0)$

M-B Indices for planes in HCP



M-B Indices for planes in HCP

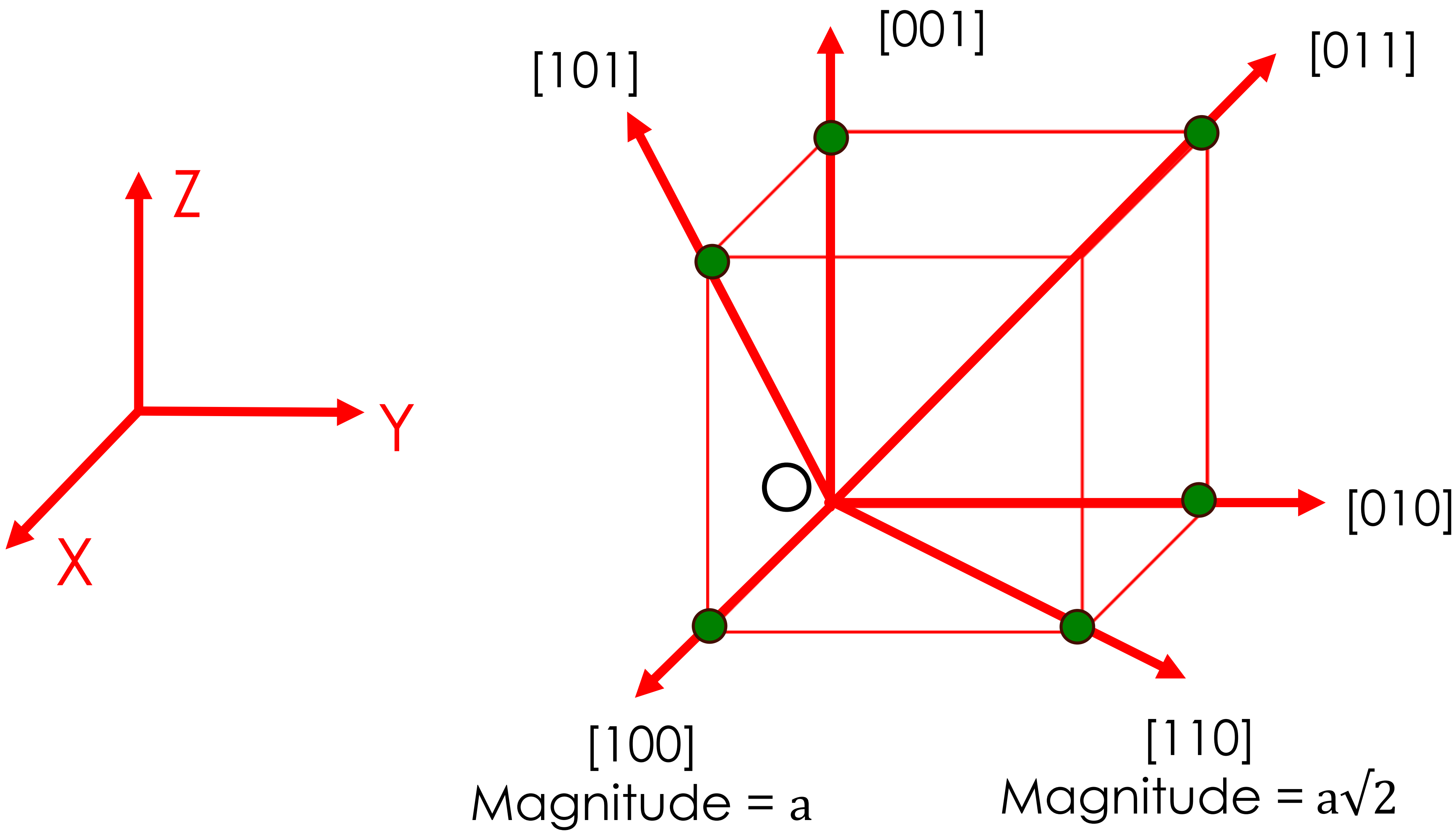




Directions in Hexagonal close-packed system

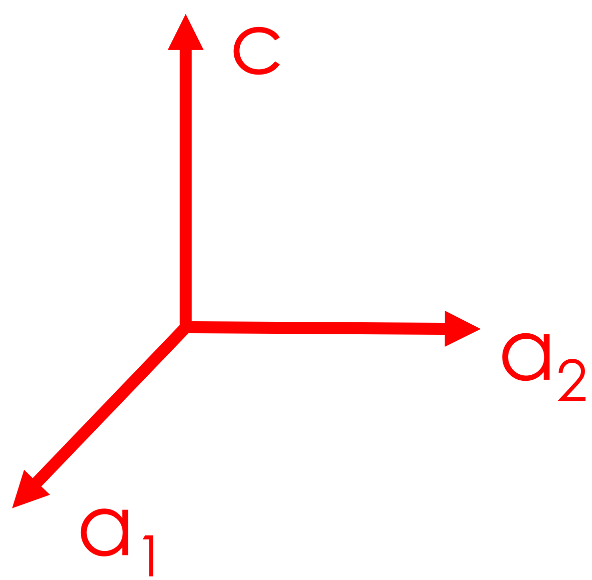
Symmetry in cubic lattice

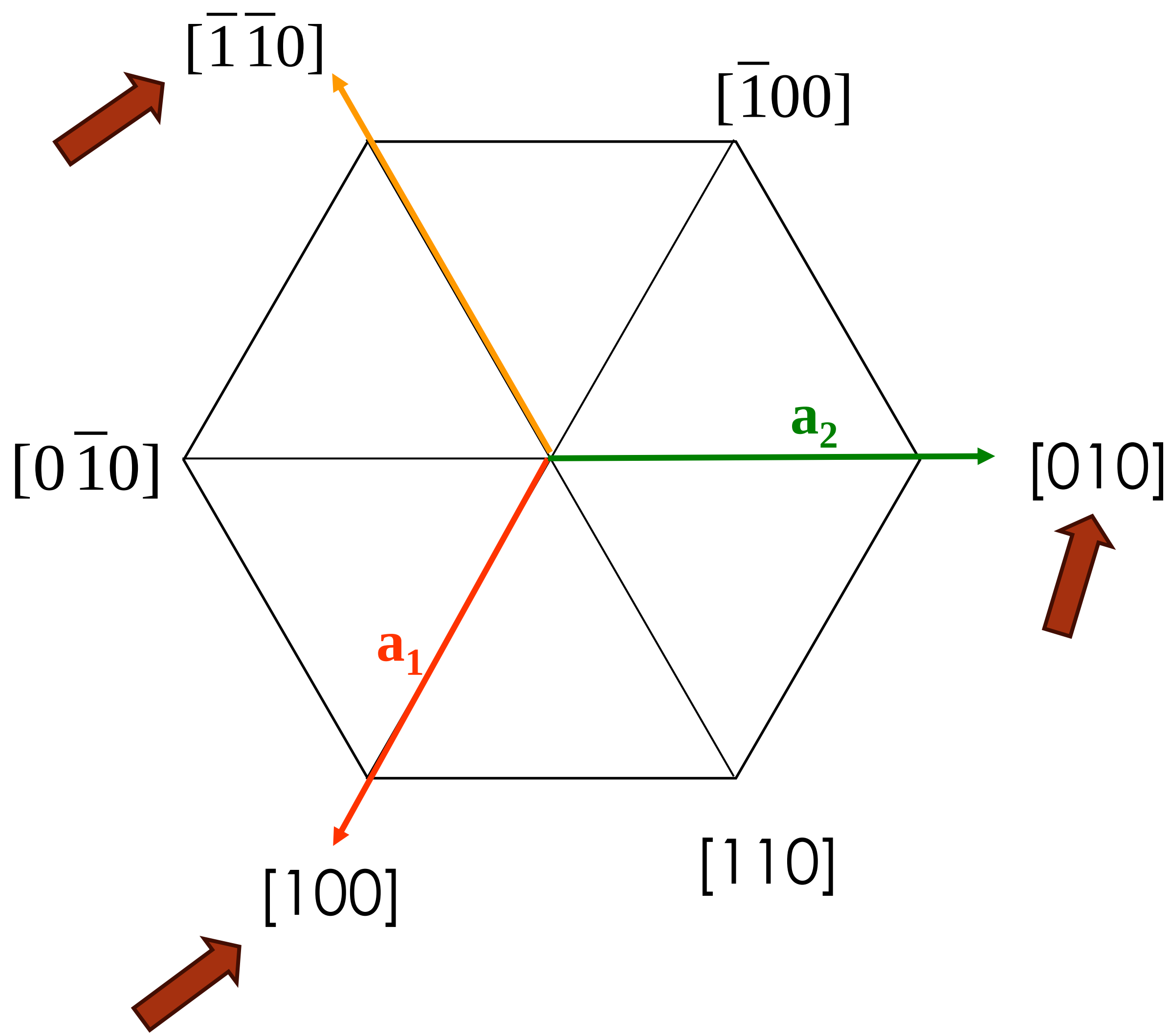
Members of the same family have the same magnitude!



Why 4 index system is needed?

Symmetry is not maintained in 3 index system.





Not from the same family of directions.

So, we may need new index system for symmetry

Derivation for the transformation formulas

$a_1*u + a_2*v + a_3*t + c*w = a_1*U + a_2*V + a_3*C$

$a_1*u + a_2*v - (a_1+a_2)*t + c*w = a_1*U + a_2*V + a_3*C$

$a_1 (u-t) + a_2 (v-t) + c*w = a_1*U + a_2*V + a_3*C$

Since $a_1 + a_2 + a_3 = 0$ ....(1) and

$u + v + t = 0$ ....(2)

This gives

$U = u - t$ ....(3)

$V = v - t$ ....(4)

$W = w$

Put the value of t in equations (3) and (4) gives

$U = 2u + v$

$V = 2v + u$

By solving the above, we get

$$u = \frac{1}{3}(2U - V)$$

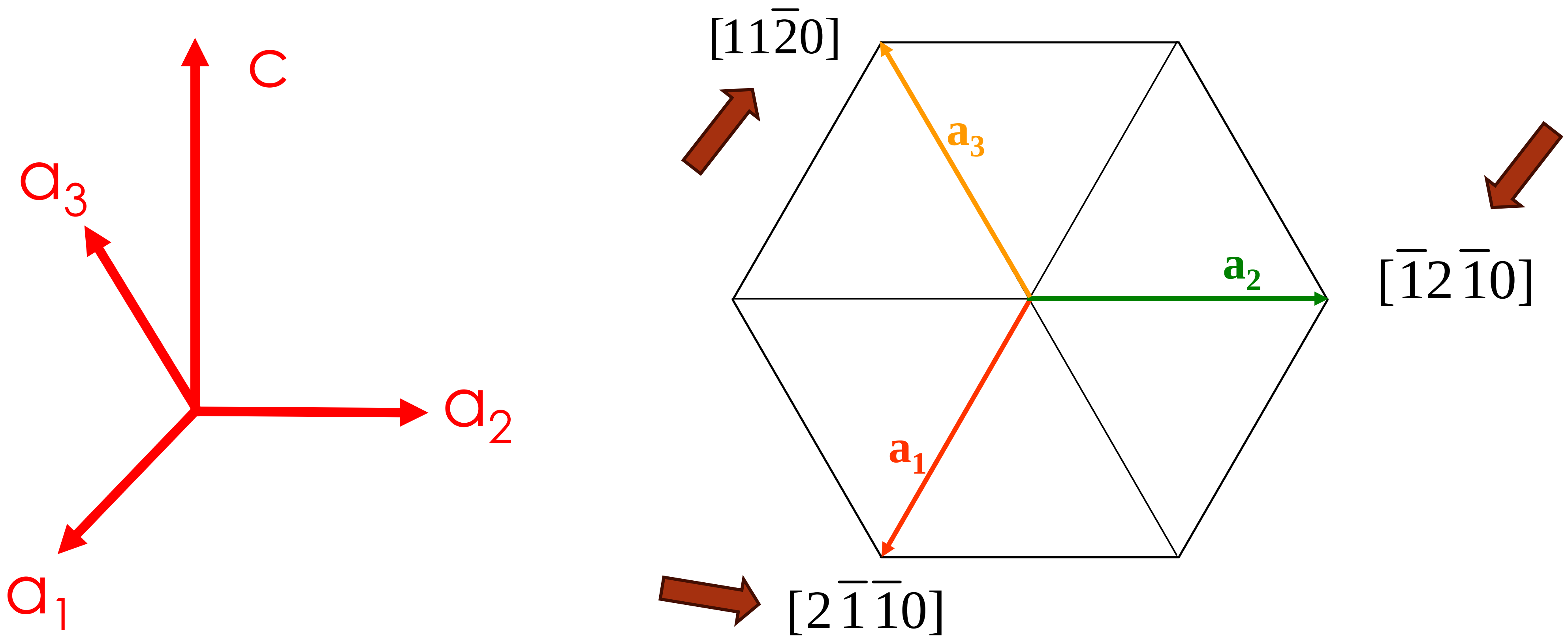
$$v = \frac{1}{3}(2V - U)$$

$$t = -(u + v)$$

$$w = W$$

Why 4 index system is needed?

Symmetry is maintained due to the extra index.



Belongs to the same family of directions.

In the three-index notation, equivalent directions may not seem equivalent, while in the four-index notation, the equivalence is brought out.

M-B Indices for direction in HCP

1. For simplicity, we will use Miller indices [UVW] for directions. (3 coordinate system)
2. We will convert Miller- Bravais notation (*uvtw*, HCP system) into MI indices (UVW) and vice a versa
3. Represent the direction as per MI indices

M-B [*uvtw*] indices from MI [UVW]	MI [UVW] from M-B indices [*uvtw*]
$u = \frac{1}{3}(2U - V)$ $v = \frac{1}{3}(2V - U)$ $t = -(u + v)$ $w = W$	$U = u - t$ $V = v - t$ $W = w$

M-B Indices for direction in HCP

Q: Show $[11\bar{2}0]$ in the HCP unit cell.

Solution:

1) Find out the MI of given MB-indices according to the transformation formulas
2) Show direction using the transformed MI [UVW]

$$\boxed{U = u - t}$$
$$\boxed{V = v - t}$$
$$\boxed{W = w}$$

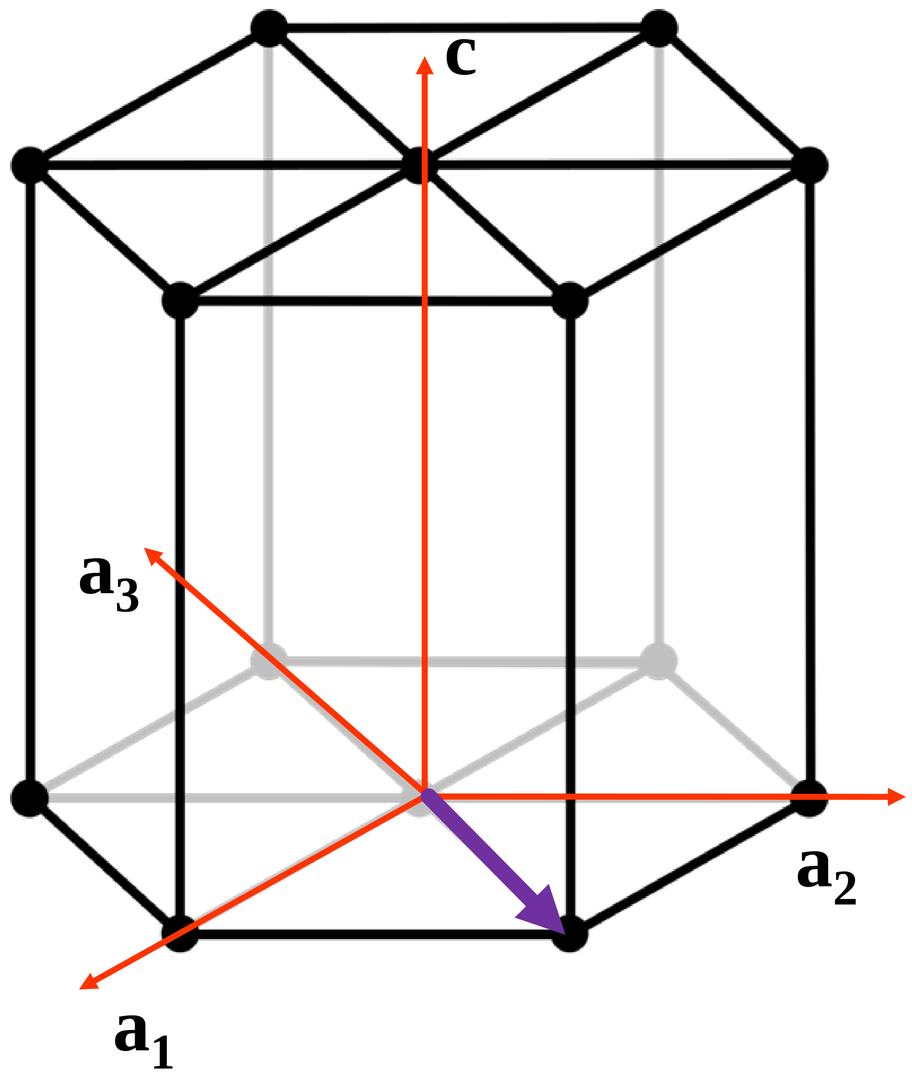
M-B Indices for direction in HCP

Show the following direction in HCP unit cell

$$[11\bar{2}0]$$

$$\boxed{U = u - t}$$
$$\boxed{V = v - t}$$
$$\boxed{W = w}$$

Steps		
1	Find out the MI using transformation formulas	[330] or [110]
2	Show direction using the transformed MI [UVW]	



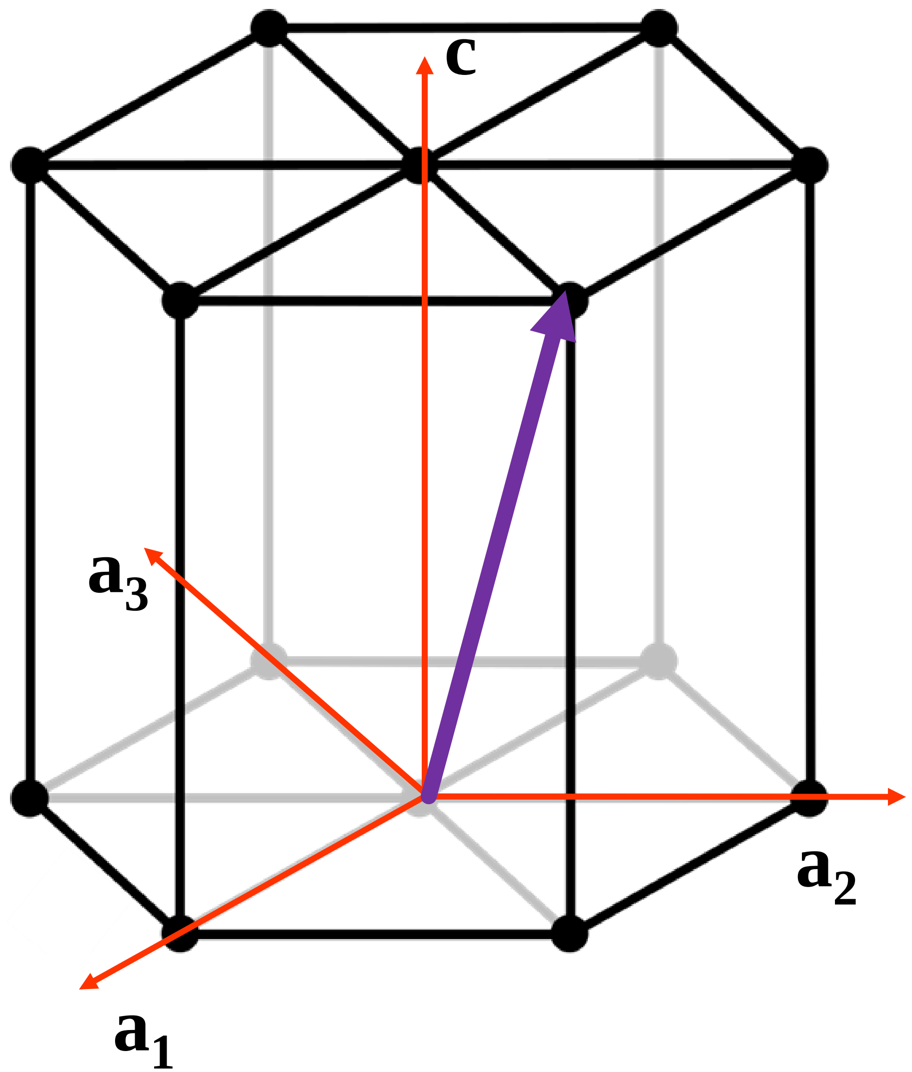
M-B Indices for direction in HCP

Show the following direction in HCP unit cell

$$[11\bar{2}3]$$

$$\boxed{U = u - t}$$
$$\boxed{V = v - t}$$
$$\boxed{W = w}$$

Steps		
1	Find out the MI using transformation formulas	[333] or [111]
2	Show direction using the transformed MI [UVW]	



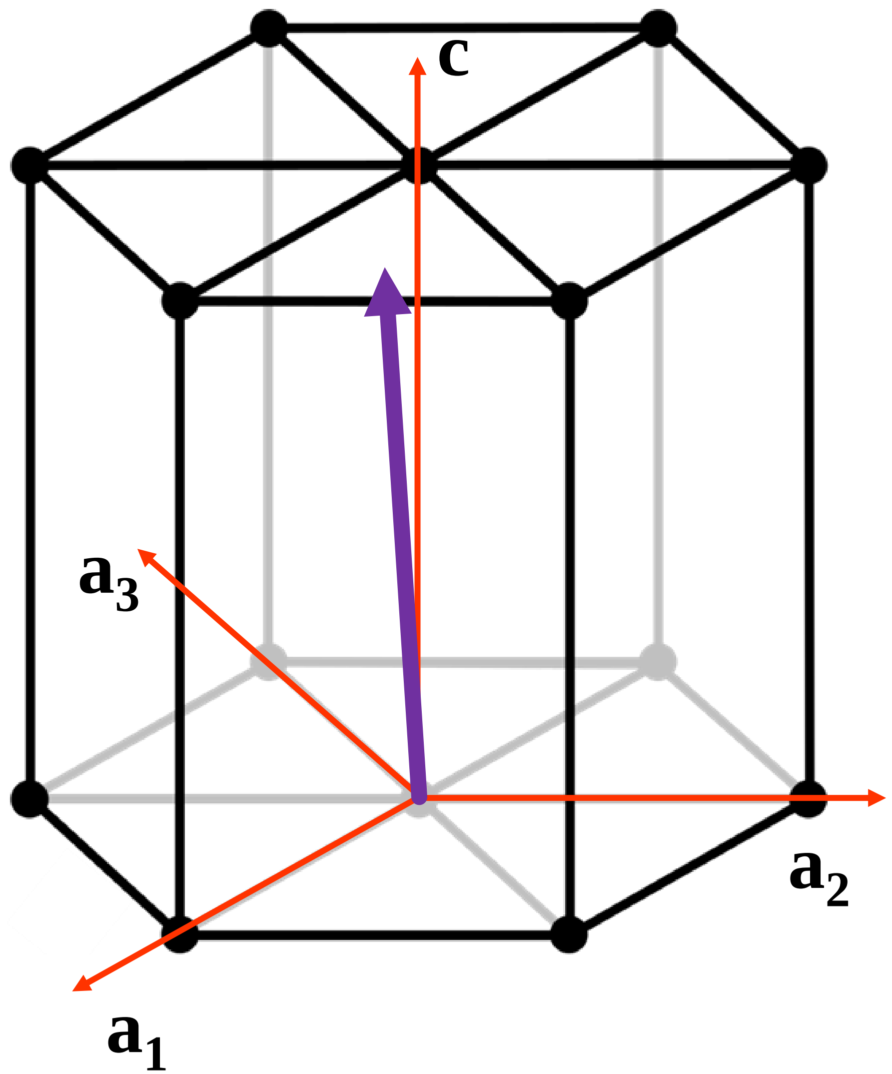
M-B Indices for direction in HCP

Show the following direction in HCP unit cell

$$[10\bar{1}3]$$

$$\boxed{U = u - t}$$
$$\boxed{V = v - t}$$
$$\boxed{W = w}$$

Steps		
1	Find out the MI using transformation formulas	[213]
2	Show direction using the transformed MI [UVW]	



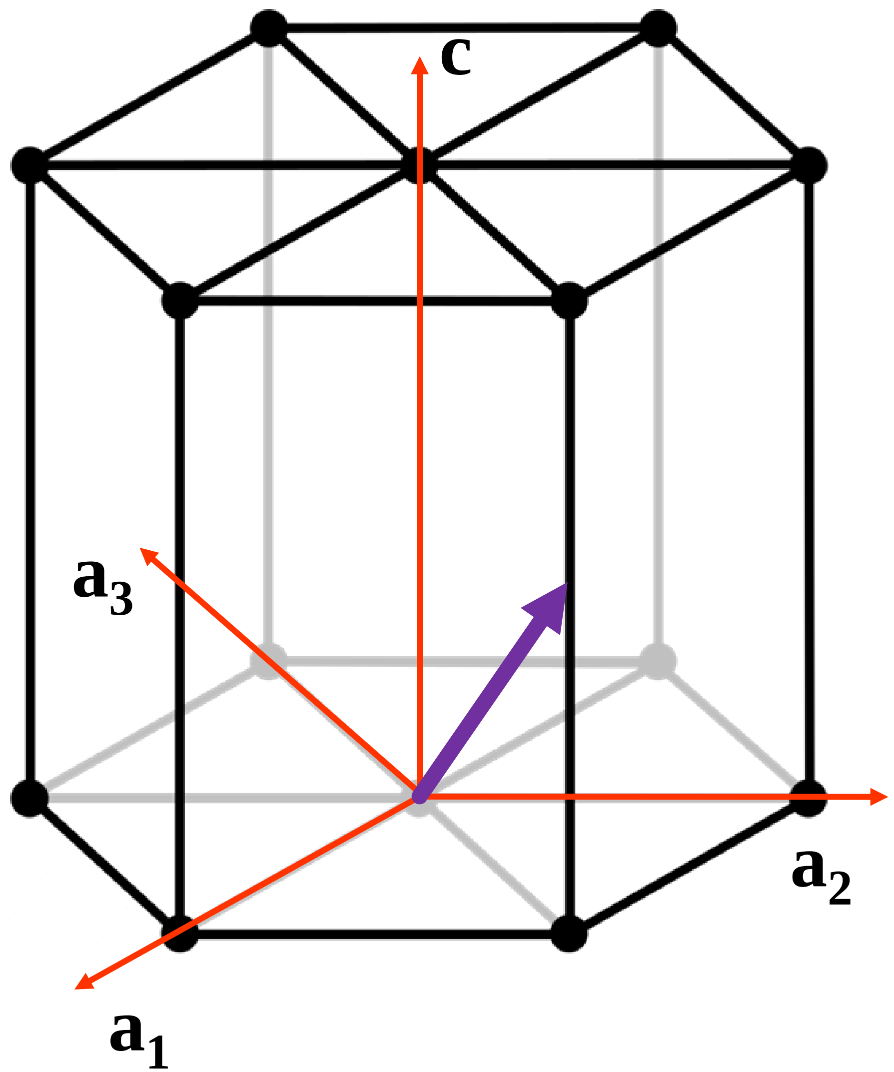
M-B Indices for direction in HCP

Show the following direction in HCP unit cell

$$[22\bar{4}3]$$

$$U = u - t$$
$$V = v - t$$
$$W = w$$

Steps		
1	Find out the MI using transformation formulas	[663] or [221]
2	Show direction using the transformed MI [UVW]	



M-B Indices for direction in HCP

When a direction is given

1) Find out the MI of the given direction
2) Convert it into the MB indices according to the transformation formulas
3) Write the MB indices for the direction

$$\boxed{u = \frac{1}{3}(2U - V)}$$

$$\boxed{v = \frac{1}{3}(2V - U)}$$

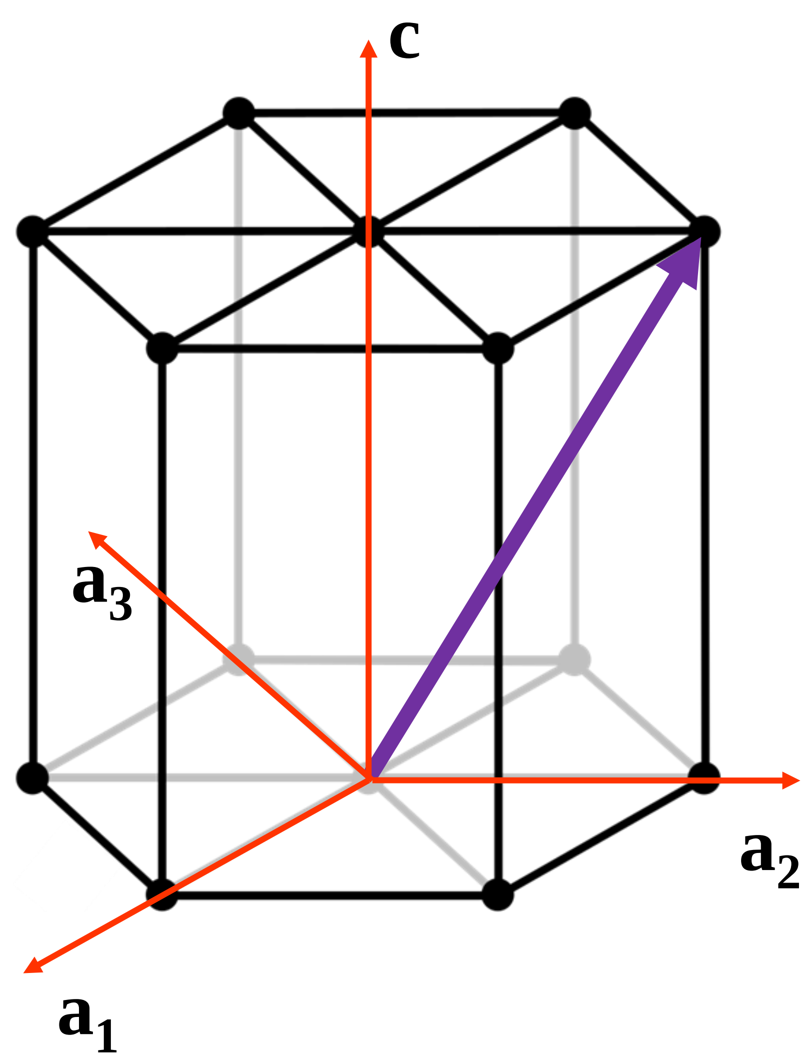
$$\boxed{t = -(u + v)}$$

$$\boxed{w = W}$$

M-B Indices for direction in HCP

Find out MB indices of a given direction

Steps		
1	Find out the MI of the given direction	[011]
2	Convert it into the MB indices according to the transformation formulas	$[\bar{1}2\bar{1}3]$



$$u = \frac{1}{3}(2U - V)$$

$$v = \frac{1}{3}(2V - U)$$

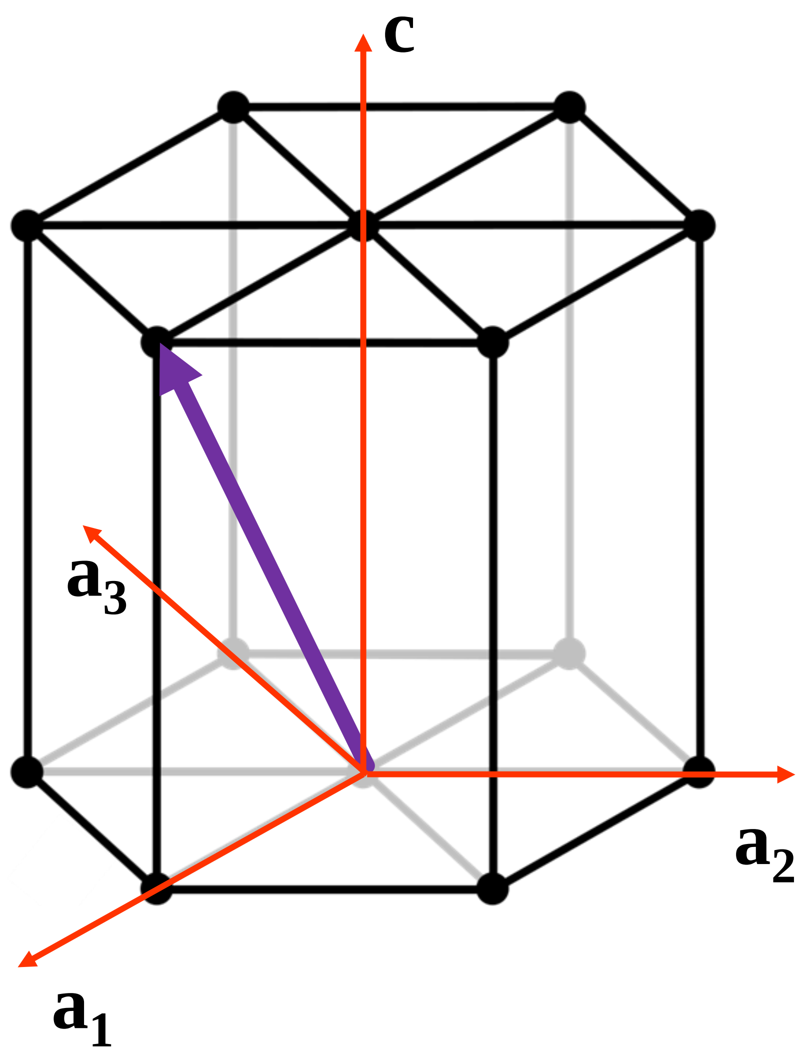
$$t = -(u + v)$$

$$w = W$$

M-B Indices for direction in HCP

Find out MB indices of a given direction

Steps		
1	Find out the MI of the given direction	[101]
2	Convert it into the MB indices according to the transformation formulas	$[2\bar{1}\bar{1}3]$



$$u = \frac{1}{3}(2U - V)$$

$$v = \frac{1}{3}(2V - U)$$

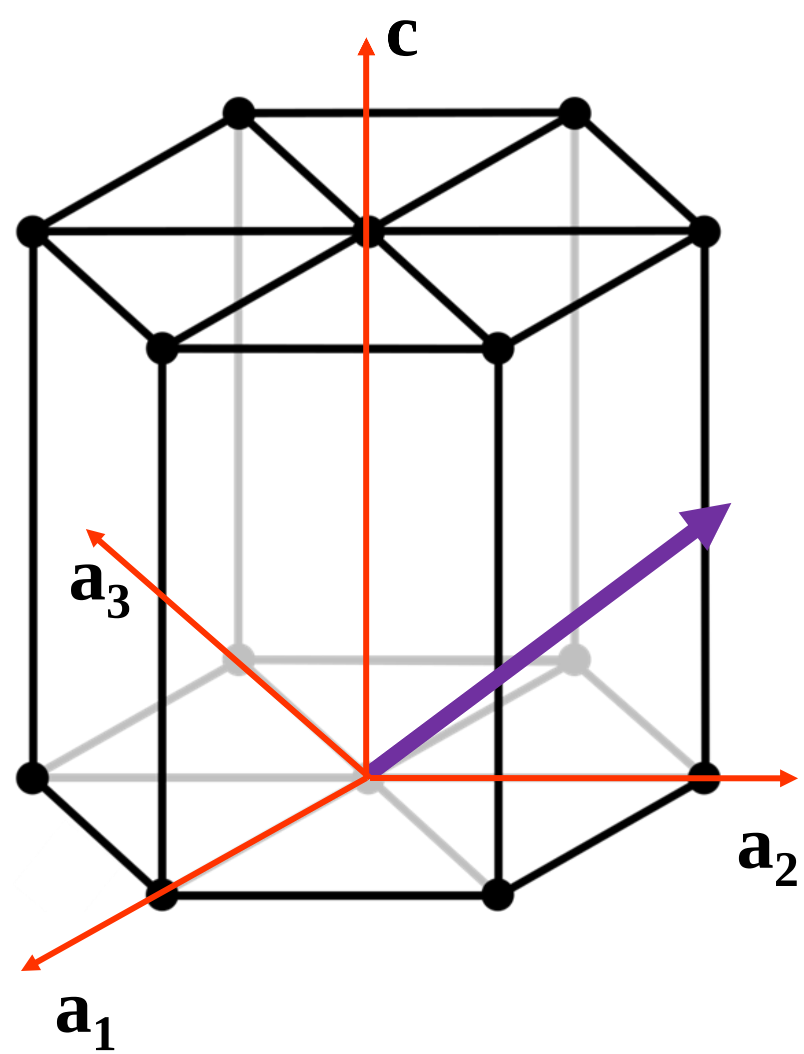
$$t = -(u + v)$$

$$w = W$$

M-B Indices for direction in HCP

Find out MB indices of a given direction

Steps		
1	Find out the MI of the given direction	[021]
2	Convert it into the MB indices according to the transformation formulas	$[\bar{2}4\bar{2}3]$



$$u = \frac{1}{3}(2U - V)$$

$$v = \frac{1}{3}(2V - U)$$

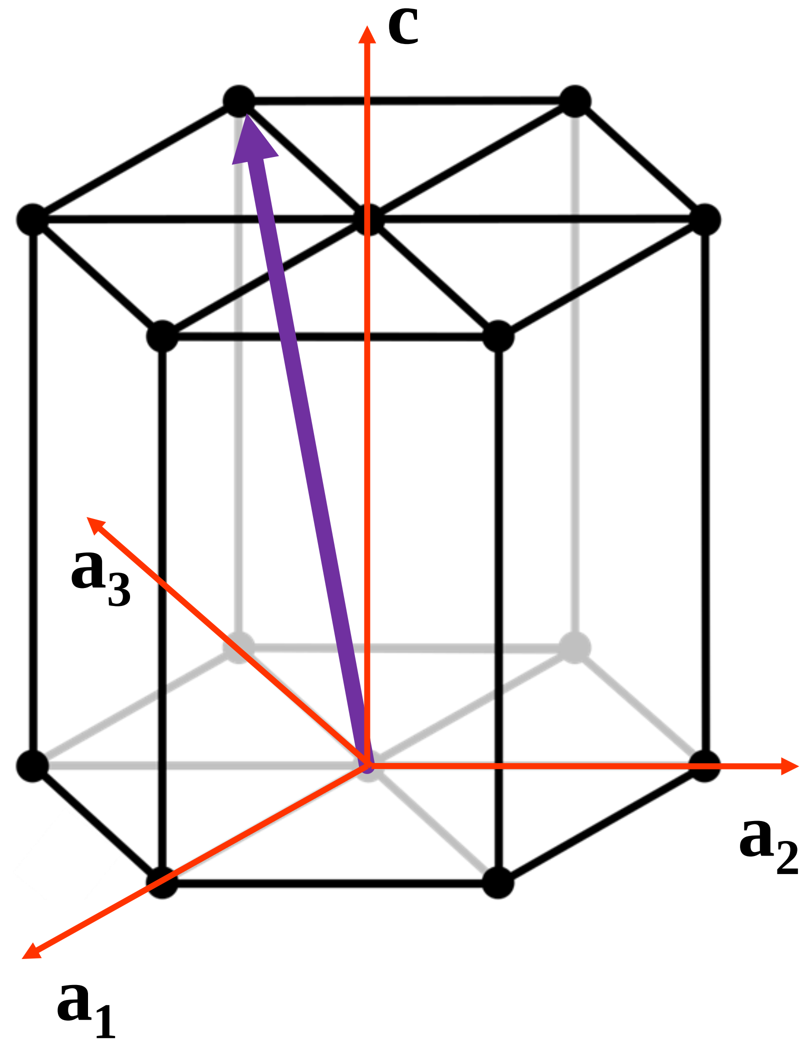
$$t = -(u + v)$$

$$w = W$$

M-B Indices for direction in HCP

Find out MB indices of a given direction

Steps		
1	Find out the MI of the given direction	$[\bar{1}11]$
2	Convert it into the MB indices according to the transformation formulas	$[\bar{1}\bar{1}23]$



$$u = \frac{1}{3}(2U - V)$$

$$v = \frac{1}{3}(2V - U)$$

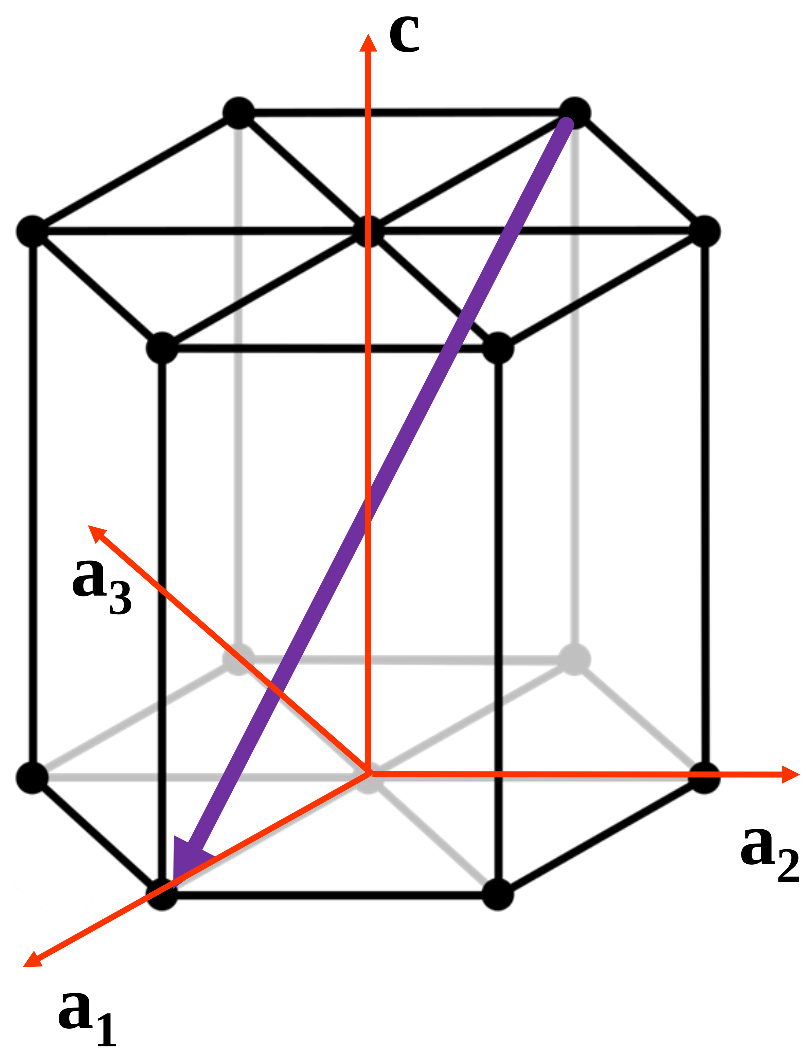
$$t = -(u + v)$$

$$w = W$$

M-B Indices for direction in HCP

Find out MB indices of a given direction

Steps		
1	Find out the MI of the given direction	$[20\bar{1}]$
2	Convert it into the MB indices according to the transformation formulas	$[4\bar{2}\bar{2}\bar{3}]$



$$u = \frac{1}{3}(2U - V)$$

$$v = \frac{1}{3}(2V - U)$$

$$t = -(u + v)$$

$$w = W$$

Summary

1. The HCP system have 4 index system to denote planes called as Miller-Bravais system.
2. The planes in HCP can be drawn by three Miller indices only. The third Miller indices is redundant in nature. It is used for symmetry.
3. The planes on the top and bottom are called as basal planes.
4. The planes parallel to c axis are called as prism planes.
5. The planes which have intercept on the c axis are called as pyramidal planes.
6. HCP has highest packing density ~ 74%
7. Ideal c/a ratio for HCP is 1.63