Hexagonal closed packed structure

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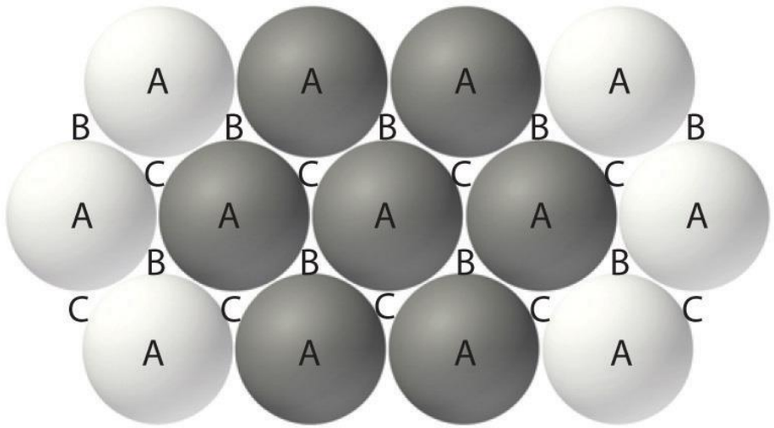
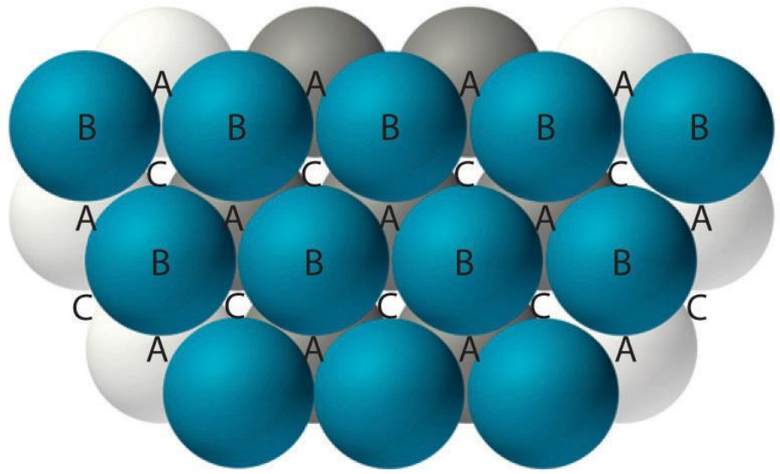
Closed packed structures

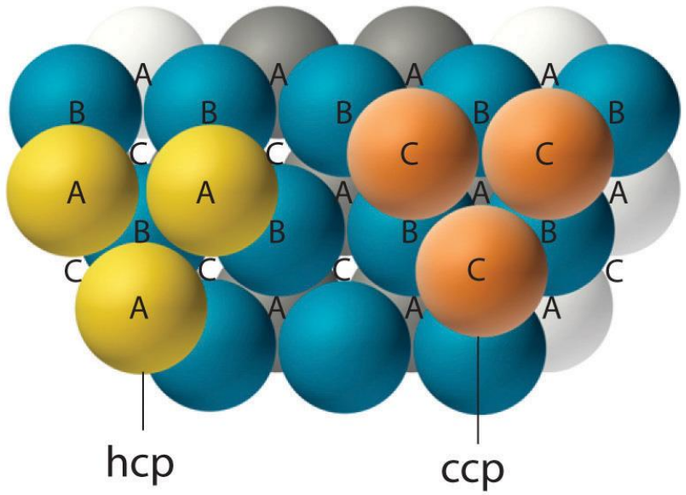
Closed packed structures have highest density in a unit cell



(a) Single layer



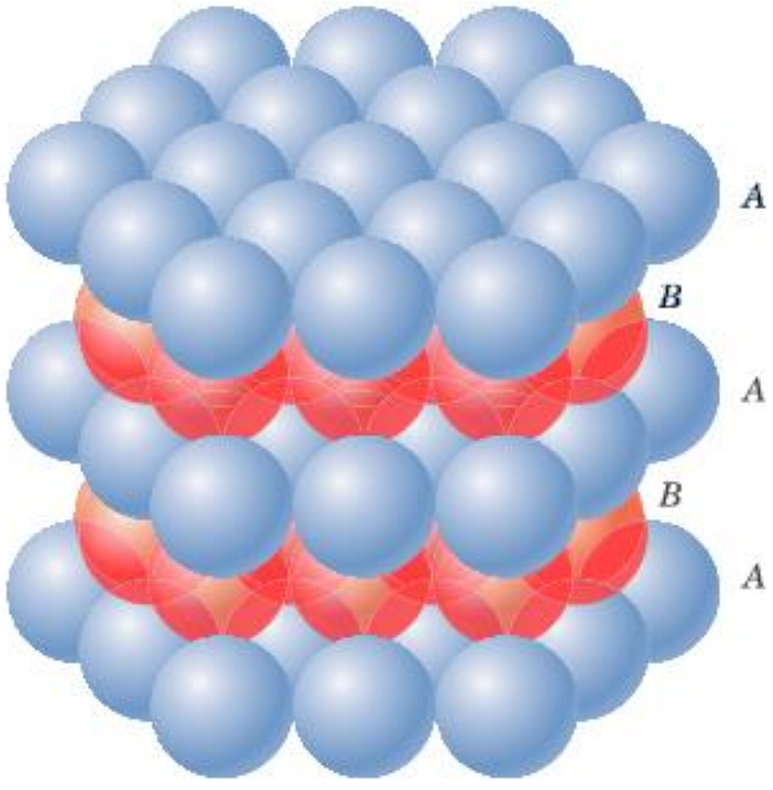
(b) Two layers

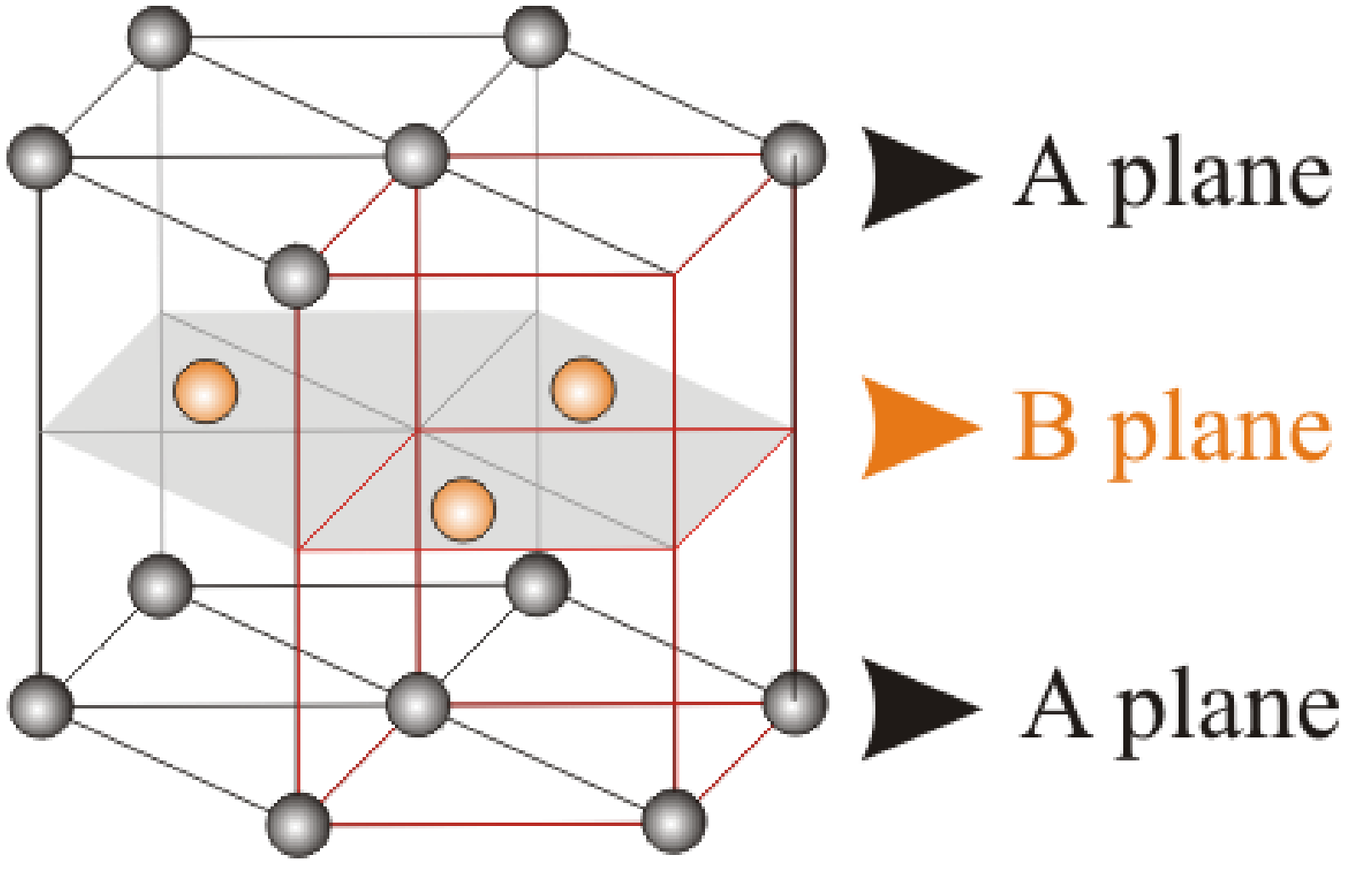


(c) Three layers

Hexagonal closed packed cubic (HCP)

HCP is a closed packed structures

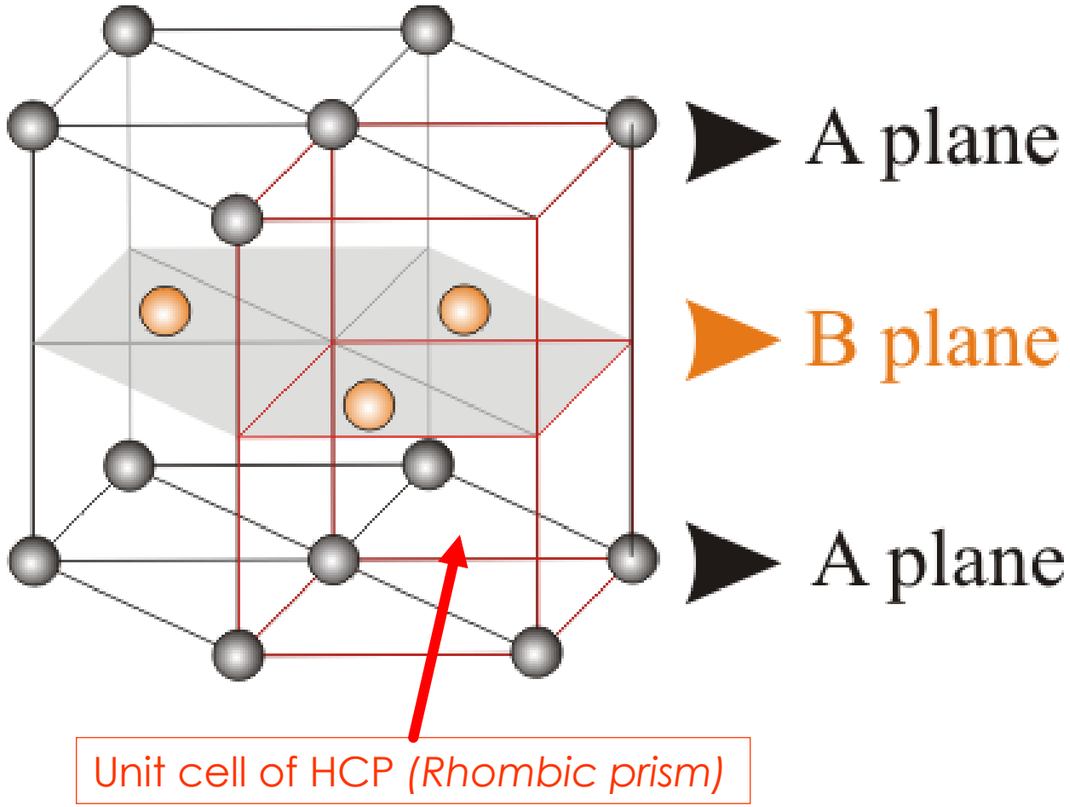


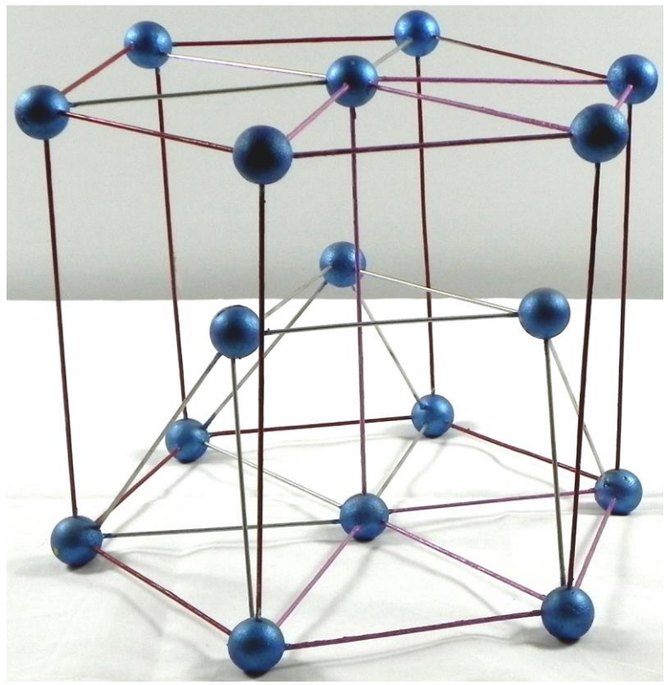


Showing 3 unit cells and the rhombic prism UC

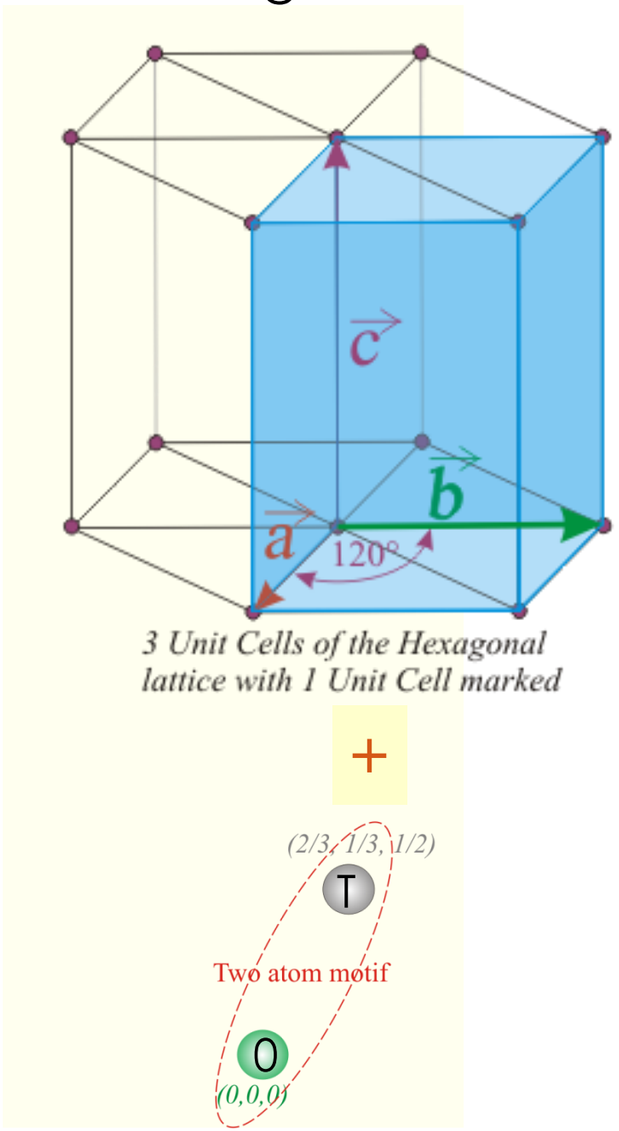
Hexagonal closed packed structure

Conventional unit cell *Showing 3 unit cells and the rhombic prism UC*





Hexagonal Lattice

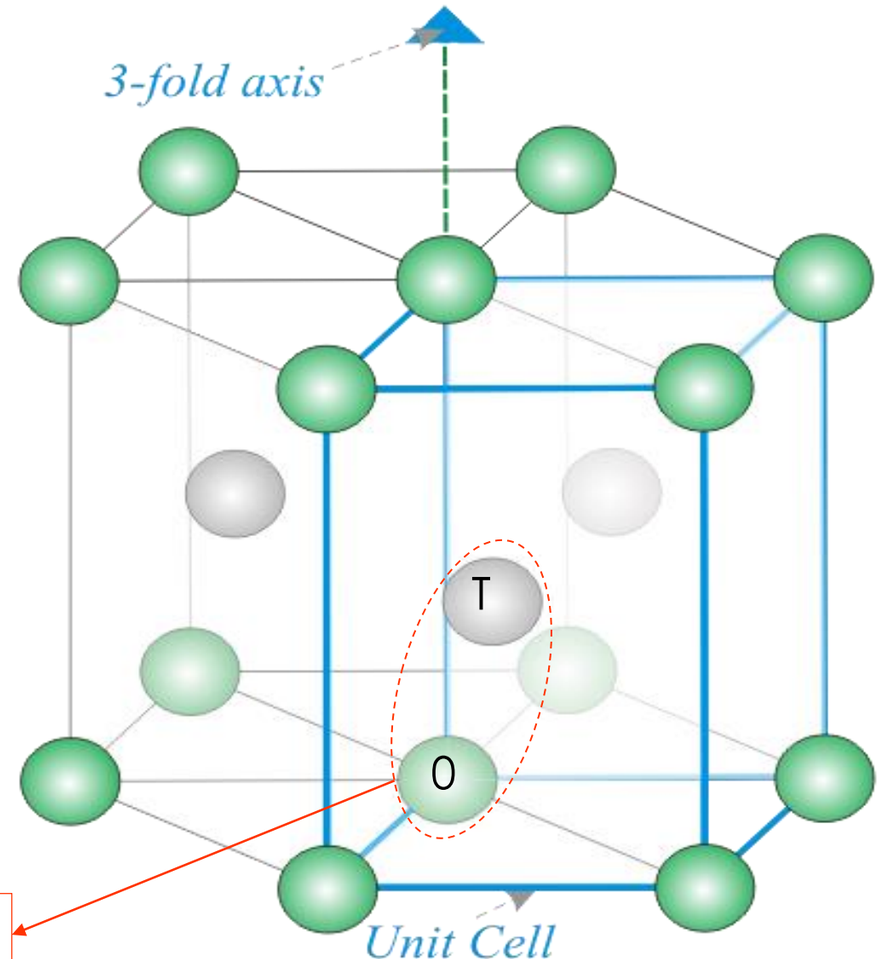


Two atom Motif

=

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

HCP crystal



Miller-Bravais index notations in HCP

- Directions and planes in hexagonal lattices and crystals are designated by the 4-index Miller-Bravais notation.
- In the four index 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 numbers which are identical
  - ➢ the fourth index represents the 'c' axis *(⊥ to the basal plane)*.

Miller-Bravais index notations in HCP

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

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

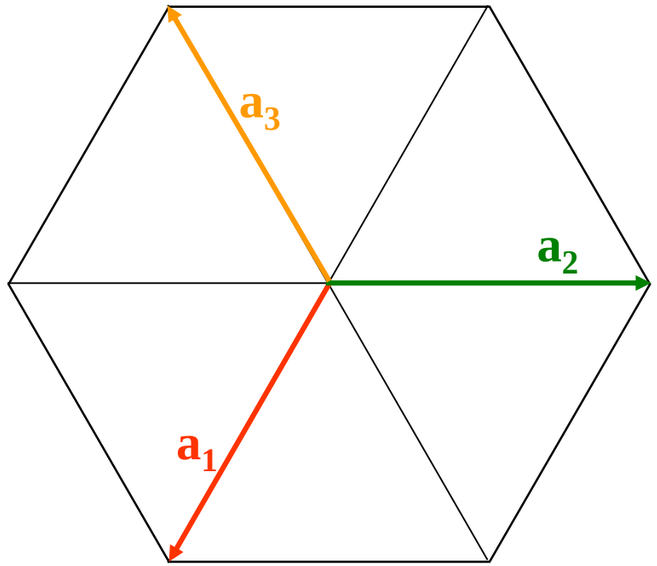
$$\mathbf{i = -(h + k)}$$

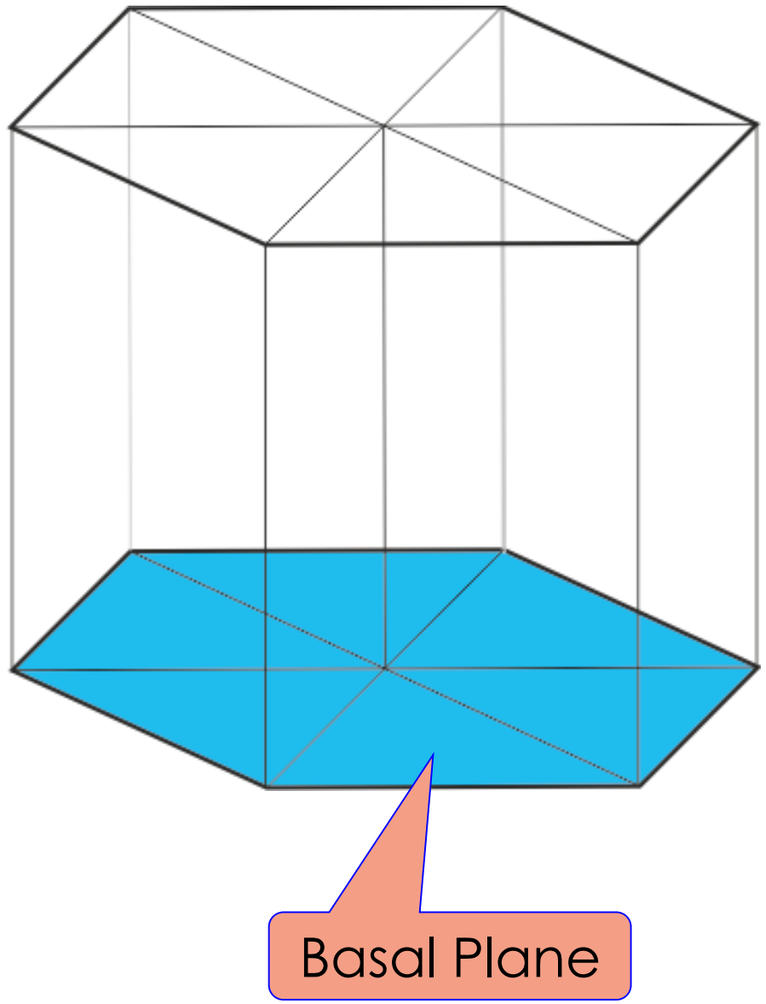
(hkl) ➔ (hkil)

(110) ➔ $(11\bar{2}0)$

MI for planes in HCP

Basal Plane



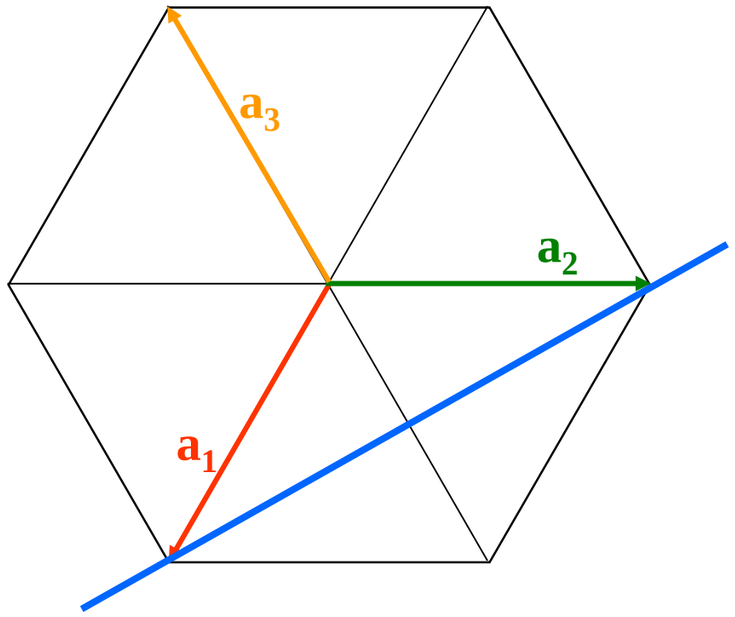


Intercepts → ∞ ∞ ∞ 1

Plane → (0 0 0 1)

MI for planes in HCP

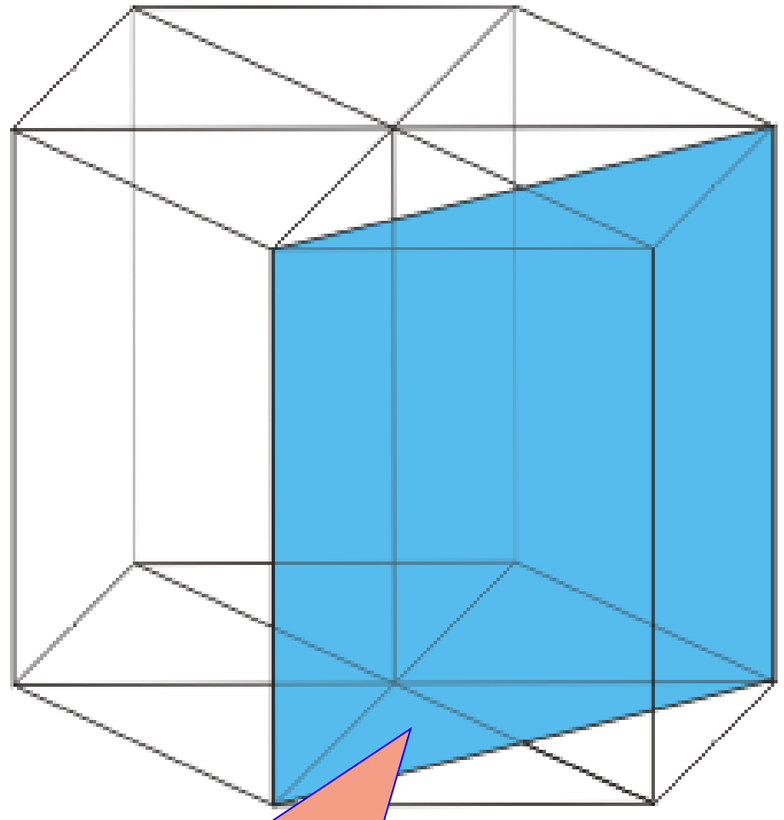
Prism planes



(h k i l)
i = –(h + k)

Intercepts → 1 1 - ½ ∞

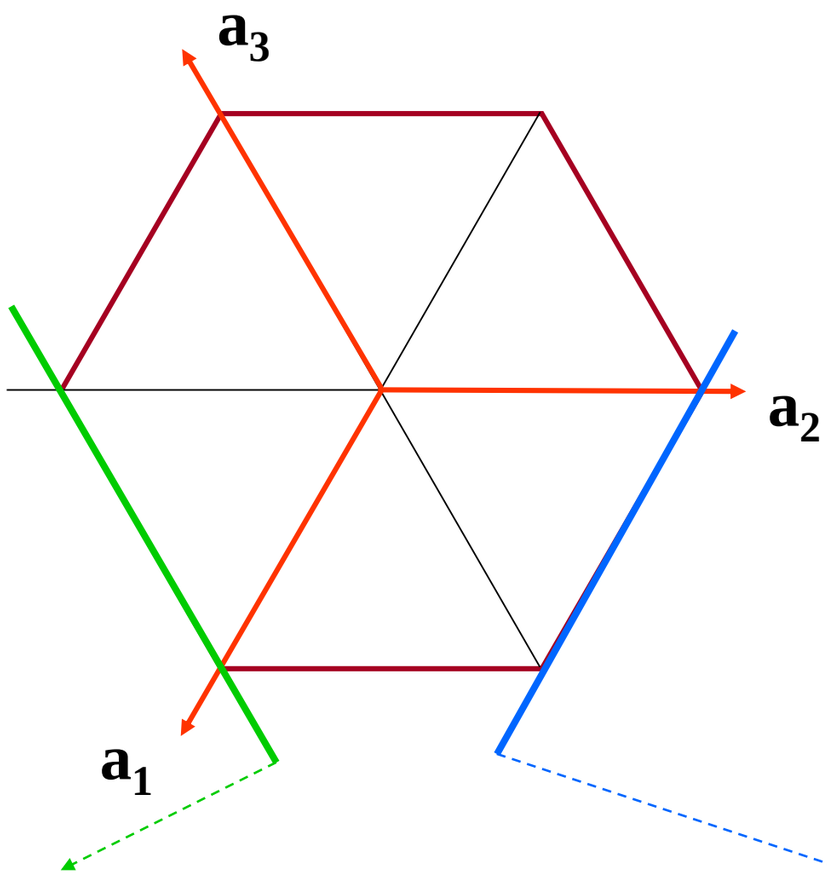
Plane → (1 1 $\bar{2}$ 0)

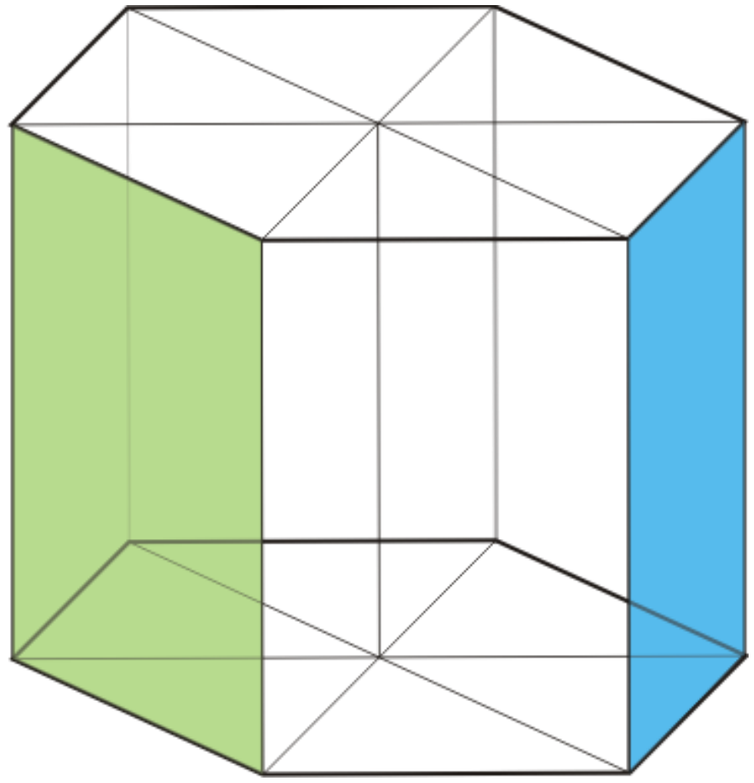


Planes which have ∞ intercept along c-axis (i.e. vertical planes) are called Prism planes

MI for planes in HCP

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





Intercepts → 1 –1 ∞ ∞

Miller → (1 $\bar{1}$ 0)

Miller-Bravais → (1 $\bar{1}$ 0 0)

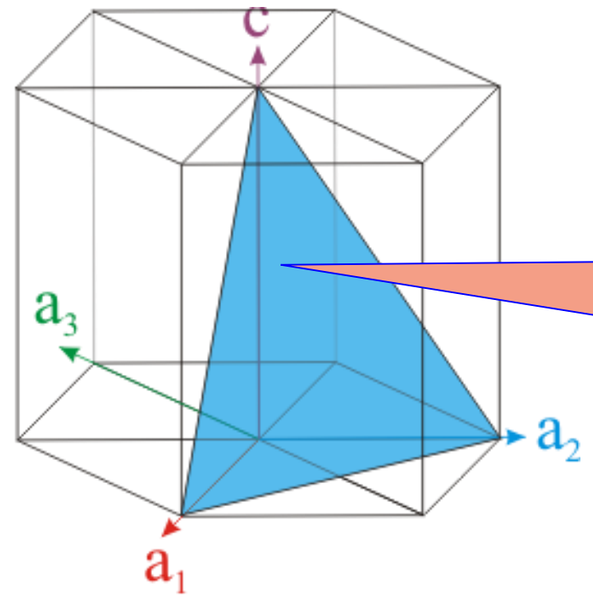
Intercepts → ∞ 1 –1 ∞

Miller → (0 1 0)

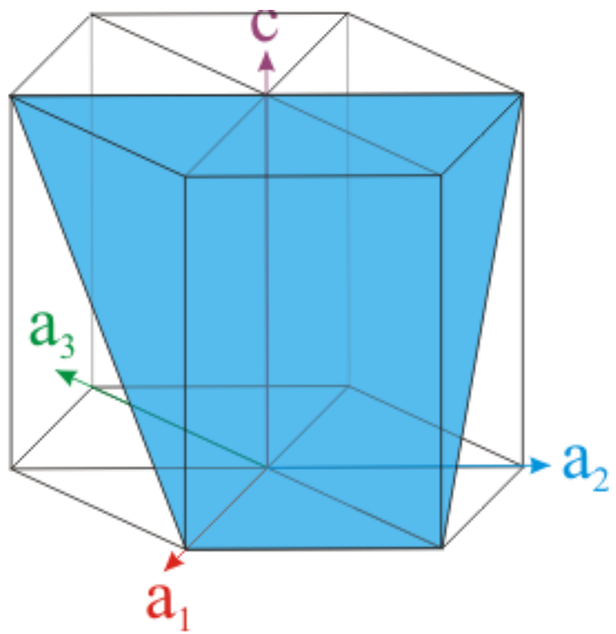
Miller-Bravais → (0 1 $\bar{1}$ 0)

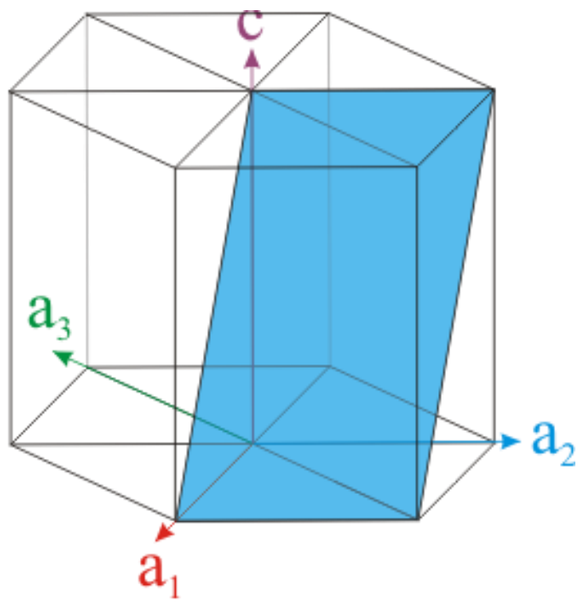
MI for planes in HCP

Pyramidal planes



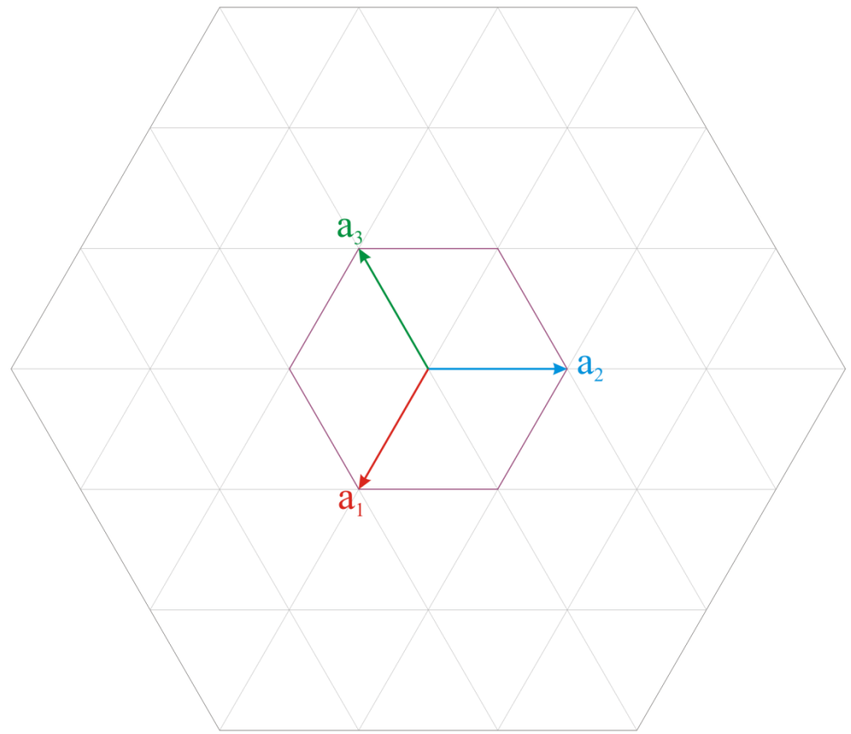
Inclined planes which have finite intercept along c-axis are called Pyramidal planes





MI for direction in HCP

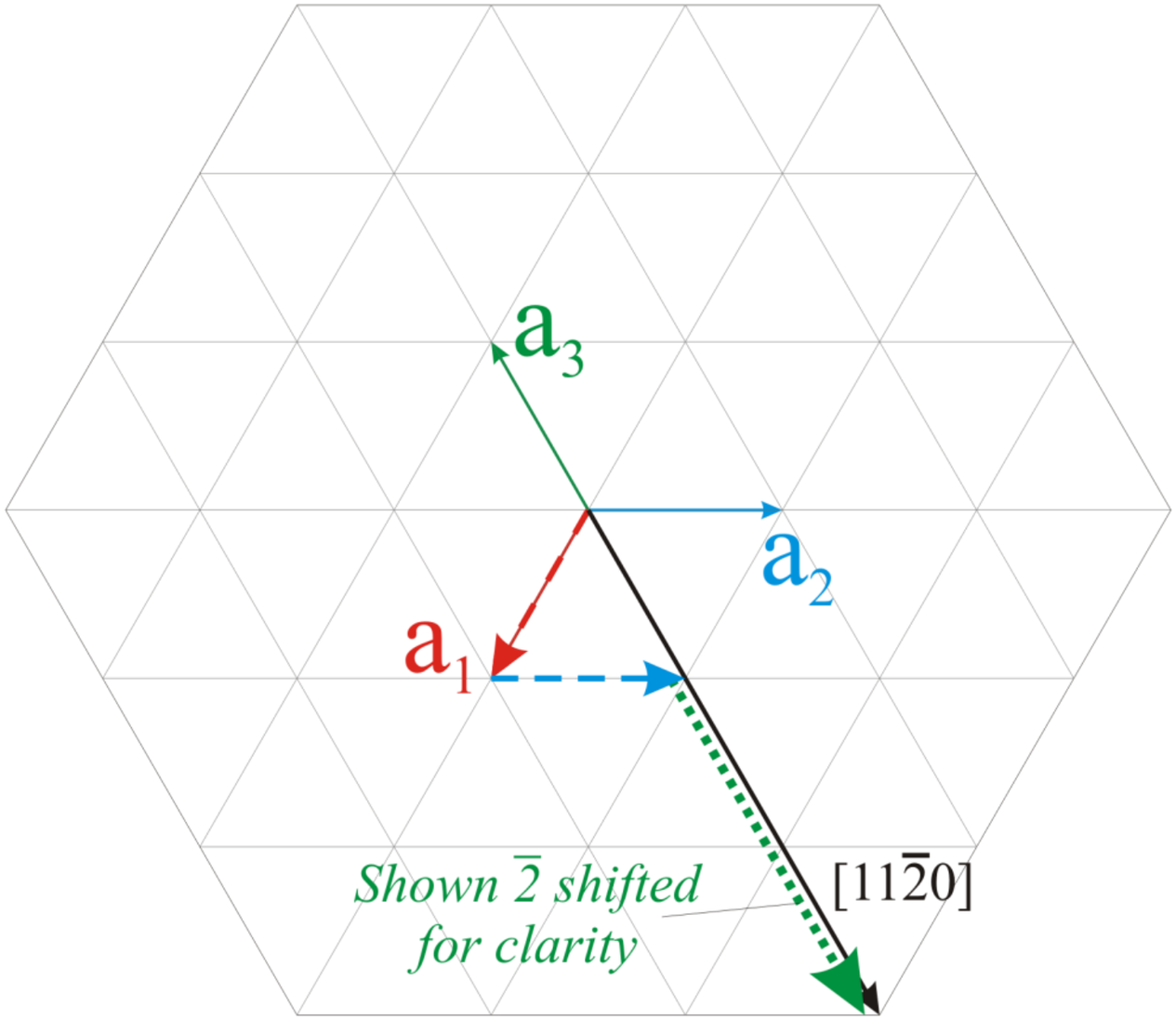
1. Basis vectors a_1, a_2 & a_3 are symmetrically related by a six fold axis.
2. The 3rd index is redundant and is included to bring out the equality between equivalent directions.
3. In the drawing of the directions we use an additional guide hexagon 3 times the unit basis vectors (a_i).



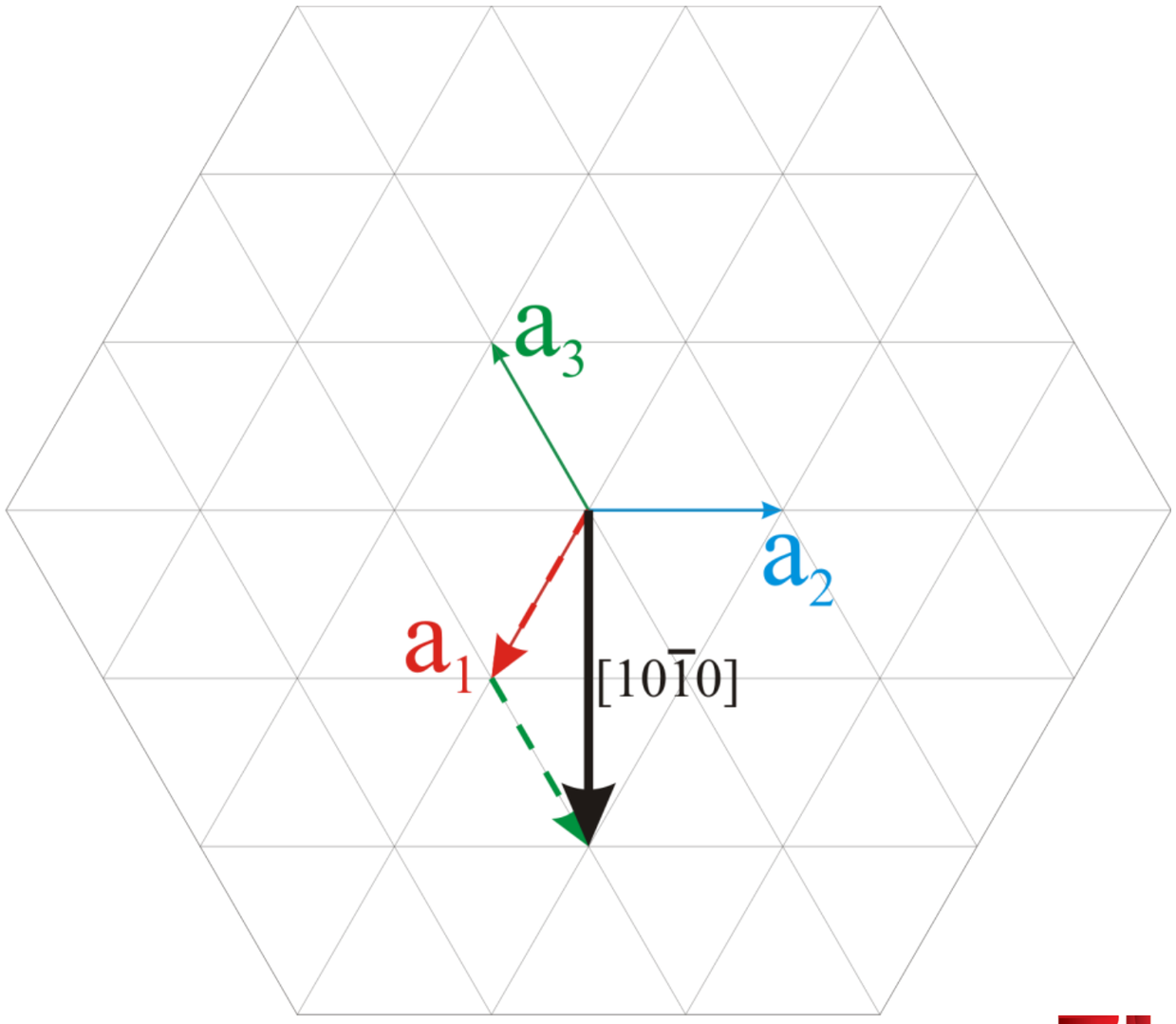
Guide Hexagon

MI for direction in HCP

Draw the [$11\bar{2}0$] direction



Draw the [$10\bar{1}0$] direction



Remember

- Only atoms whose center of mass lies on the plane has to be count.
- In the BCC crystal, the (111) plane partially intersects the atom at the body center (½,½,½). This atom has to be excluded from the calculation.

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