MLL 100

Introduction to Materials Science and Engineering

Lecture-6

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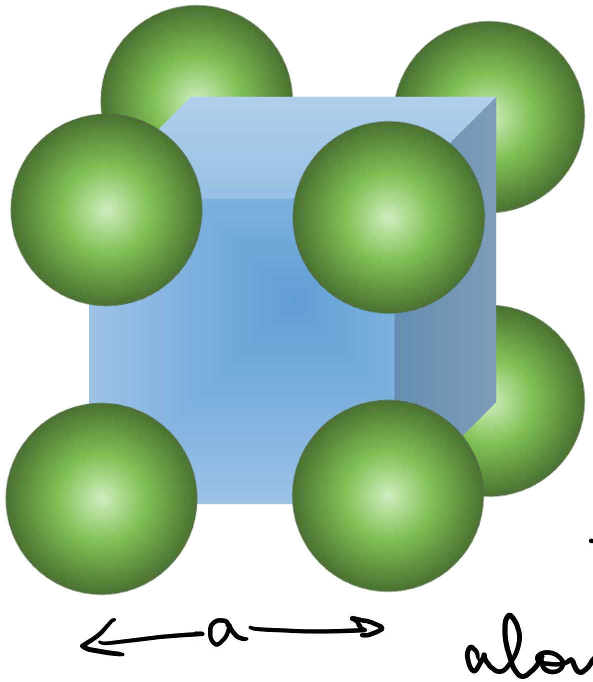
What we learnt in Lecture-5?

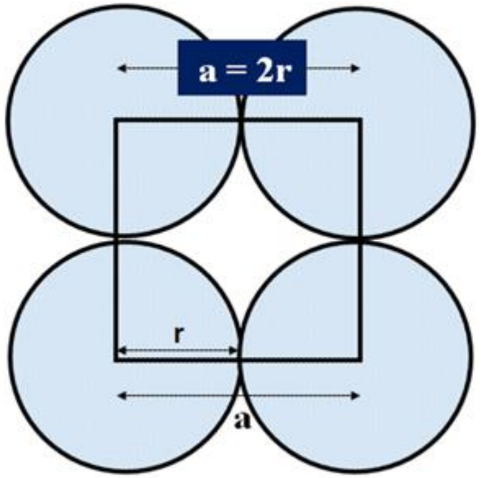
- Miller indices in cubic system

Atomic packing factor (APF): Simple Cubic



Let the radius of an atom be
and the lattice parameter
of the cubic cell be 'a'.

∴ If you consider (100);
two atoms will be in contact
along the edges (as shown in the figure)

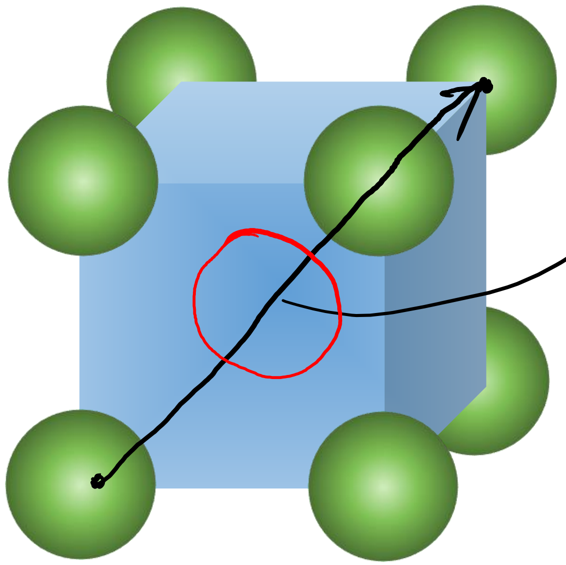


$\therefore\ 2r = a \quad \therefore\ r = \left(a/2\right)$

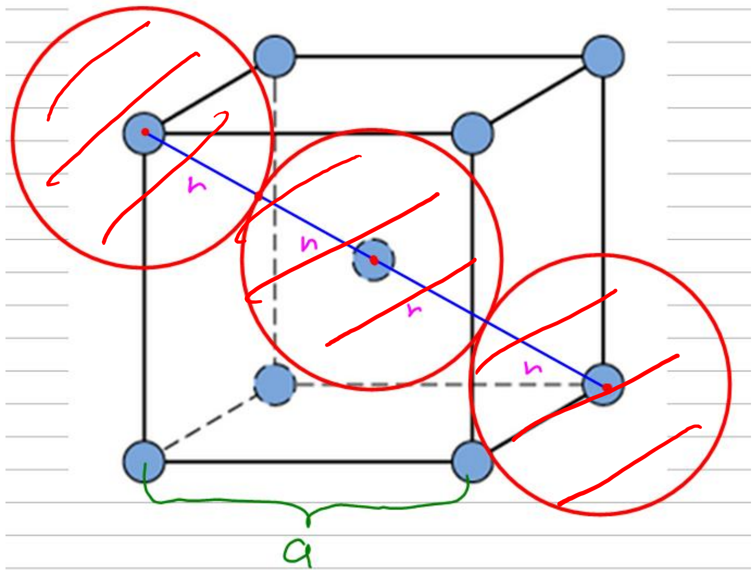
$$\therefore\ APF = \frac{\text{(No. of effective atoms (UC))} \times \text{Vol. of an atom}}{\text{Vol. of a UC}}$$

$$\therefore\ APF = \frac{1 \times \frac{4}{3}\pi r^3}{a^3} = 52\%$$

Atomic packing factor (APF): Body-centred cubic



[The atoms will be most closely packed along the body diagonal, i.e.; [1 1 1].

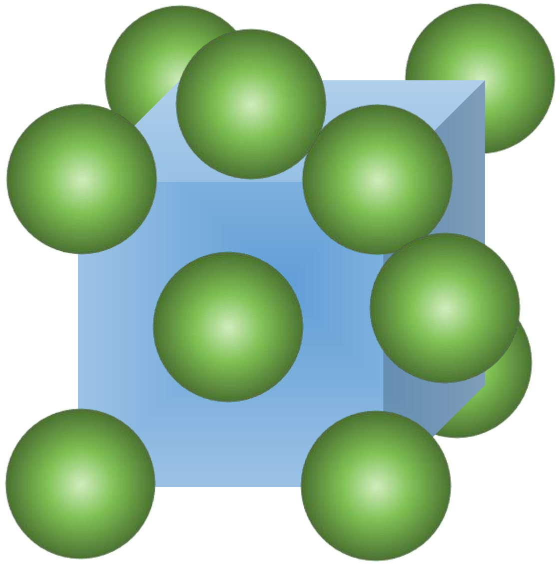


$\therefore 4r = \sqrt{3}\,a$

$r = \left(\frac{\sqrt{3}\,a}{4}\right)$

Similarly, APF $= \dfrac{2 \times \frac{4}{3}\pi\left(\frac{\sqrt{3}}{4}a\right)^3}{a^3} = \underline{\underline{68\%}}$

Atomic packing factor (APF): Face-centred cubic

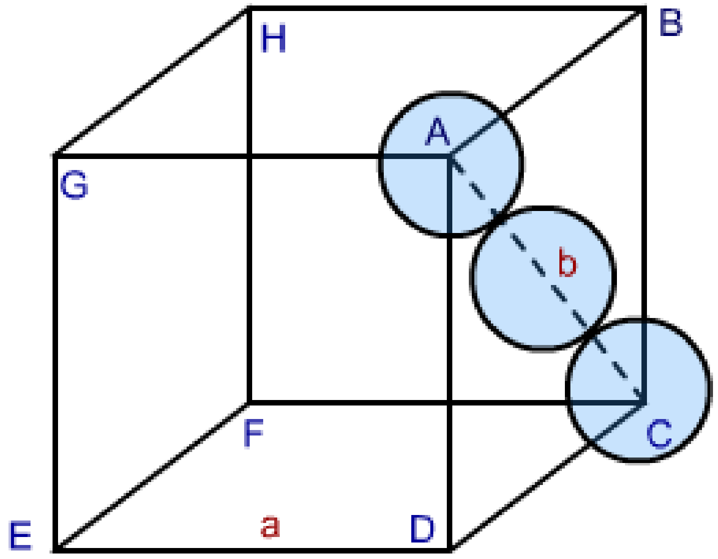


In FCC, the atoms will be closely packed along the face diagonals.

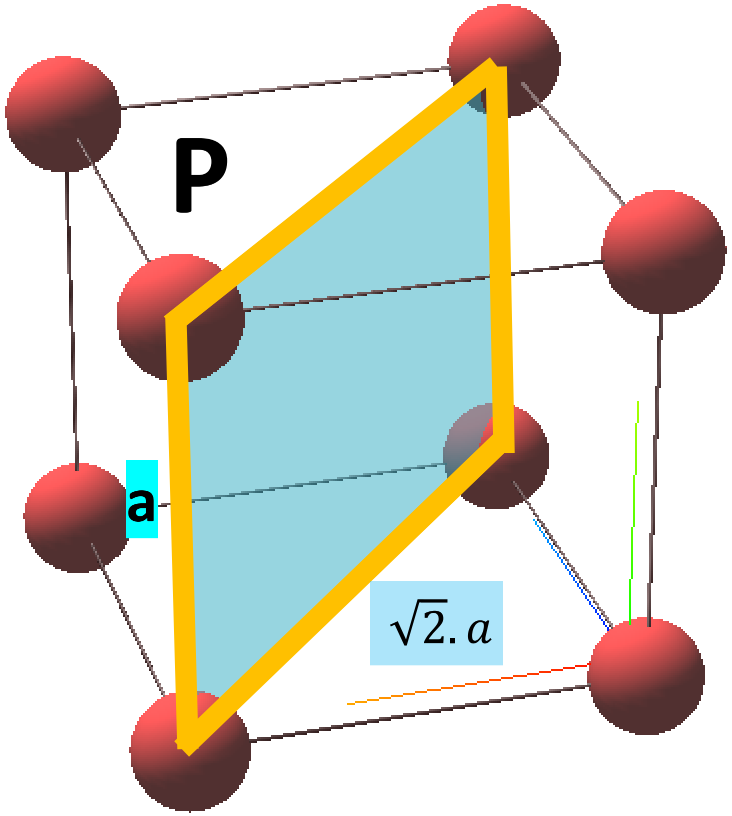
$\therefore 4r = \sqrt{2}a \quad \therefore r = \left(\frac{\sqrt{2}a}{4}\right)$

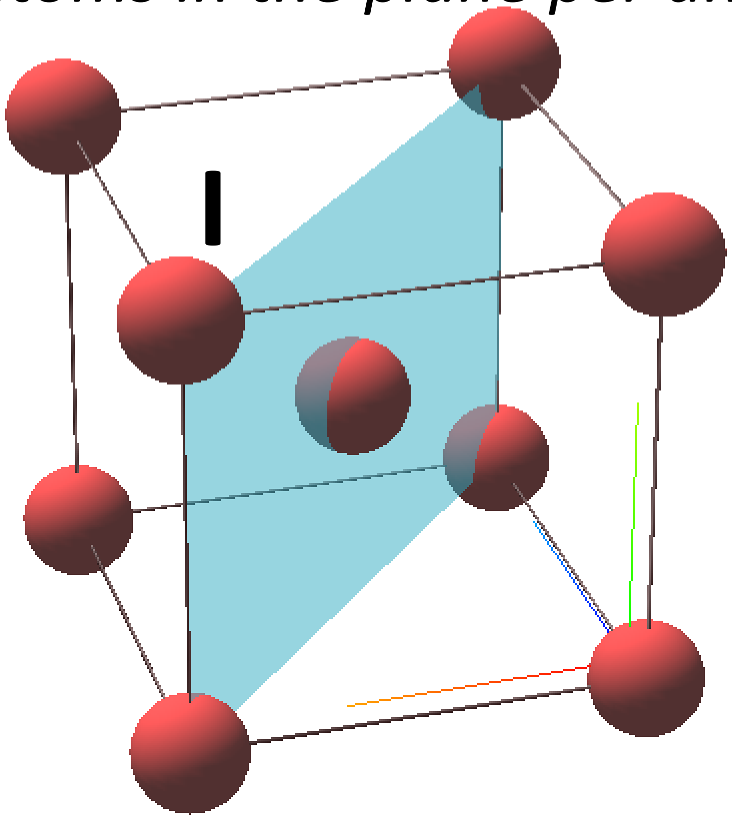
$\therefore APF = \frac{4 \times \frac{4}{3}\pi\left(\frac{\sqrt{2}a}{4}\right)^3}{a^3}$

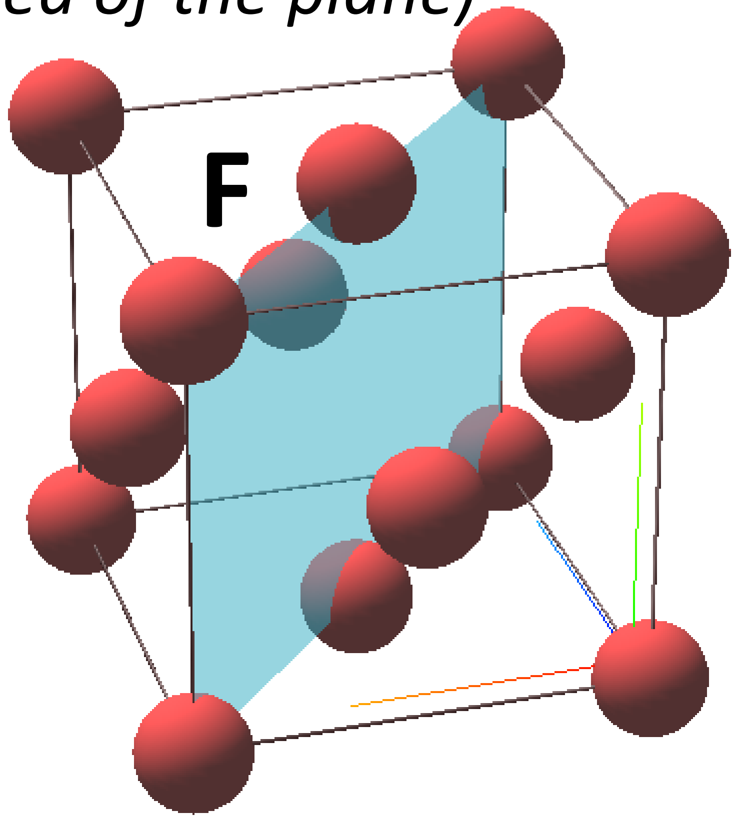
$= 74\%$.



Planar density *(No. of atoms in the plane per unit area of the plane)*







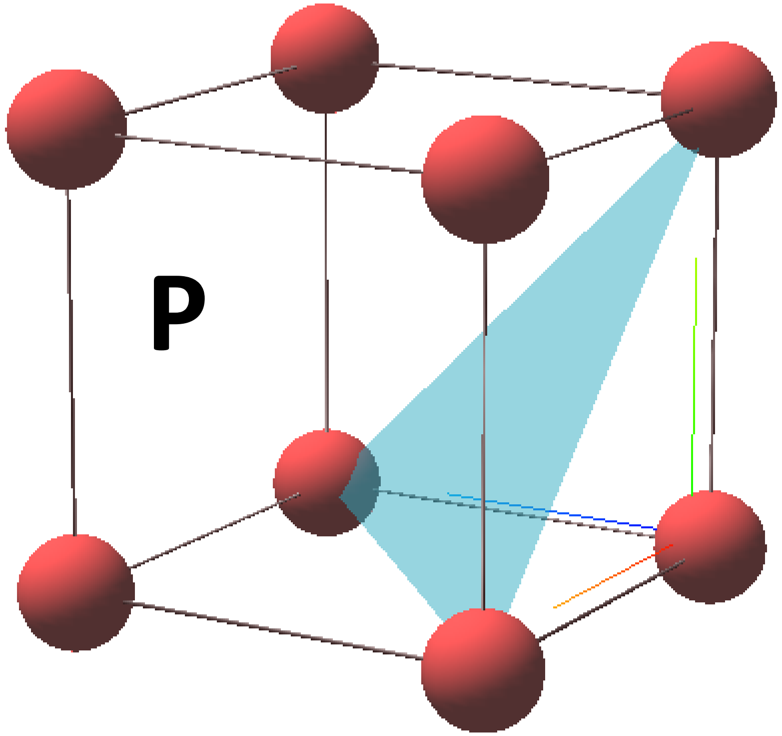
$(4)\ \mathrm{x}\ \frac{1}{4} = 1$

$[(4)\ \mathrm{x}\ \frac{1}{4}] + [(1) x\ 1] = 2$

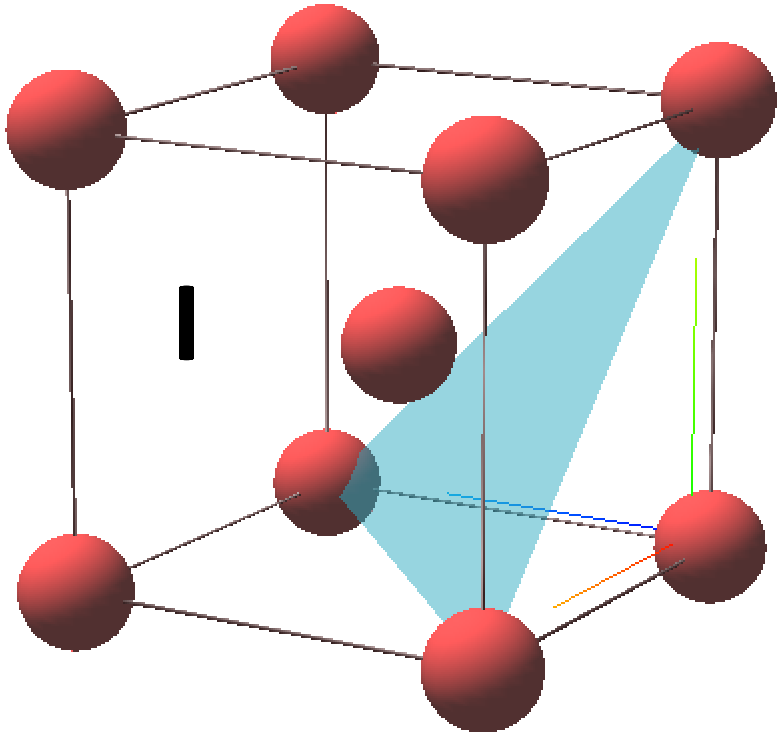
$[(4)\ \mathrm{x}\ \frac{1}{4}] + [(2) x\ \frac{1}{2}] = 2$

Area of (110) plane = a x ($\sqrt{2}.a$) = $\sqrt{2}$. a^2

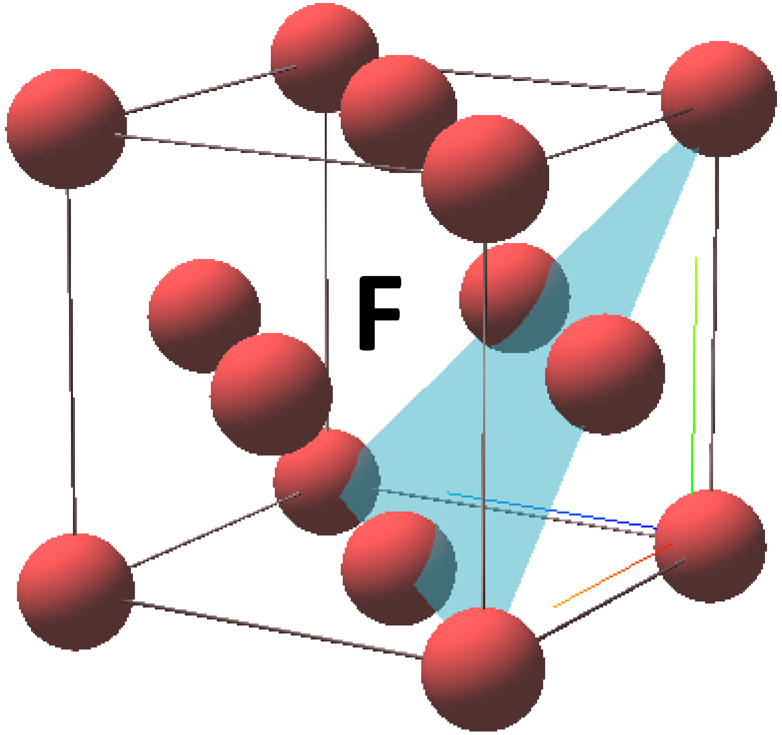
Which of the cubic Bravais lattice has the highest packing density for the (1 1 1) plane?



$(3)\ \mathrm{x}\,\frac{1}{6} = \frac{1}{2}$



$(3)\ \mathrm{x}\,\frac{1}{6} = \frac{1}{2}$



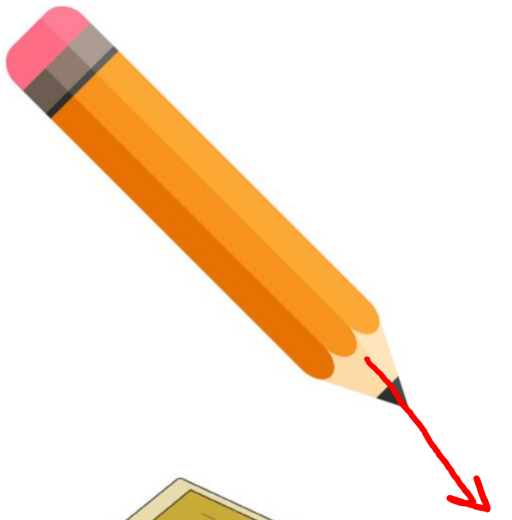
$[(3)\ \mathrm{x}\,\frac{1}{6}] + [(3)x\,\frac{1}{2}] = 2$

Area of (111) plane = $(\sqrt{3}/4.\, a^2)$ = $(\sqrt{3}/4.\, (\sqrt{2}a)2)$ = 0.866 a^2

Weiss Zone law

If a (h k l) plane lies in a zone [u v w] --------> if the [u v w] direction is || to the (h k l) plane, then:

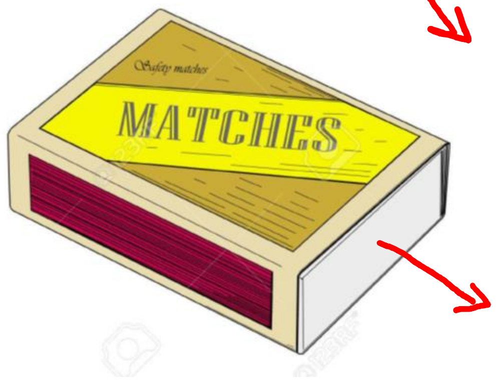
$$(hu + kv + lw) = 0$$



- ❑ Zone: a set of planes in a crystal whose intersections are all parallel.
- ❑ Zone axis: Common direction of the intersections.

- ❑ Can the directions in a crystal be called zone axes?

  …… ‘Zone axes’ and ‘directions’ are synonymous.

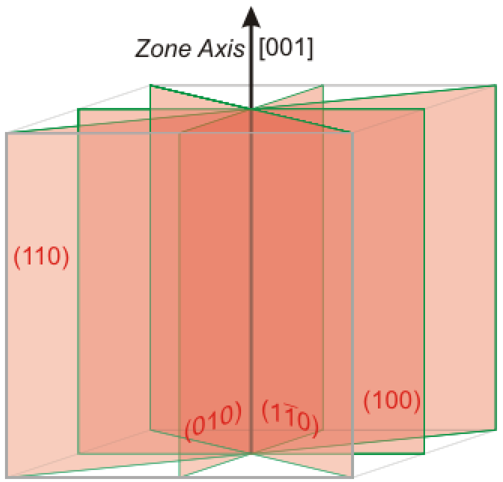


- ❑ Direction of a Pencil lead: Zone axis for all the faces enclosing it.

Zone axis at the intersection of the lattice planes

- If (h_1 k_1 l_1) & (h_2 k_2 l_2) are two planes having a common direction [u v w], according to Weiss zone law:

$$u.h_1 + v.k_1 + w.l_1 = 0 \; \& \; u.h_2 + v.k_2 + w.l_2 = 0$$

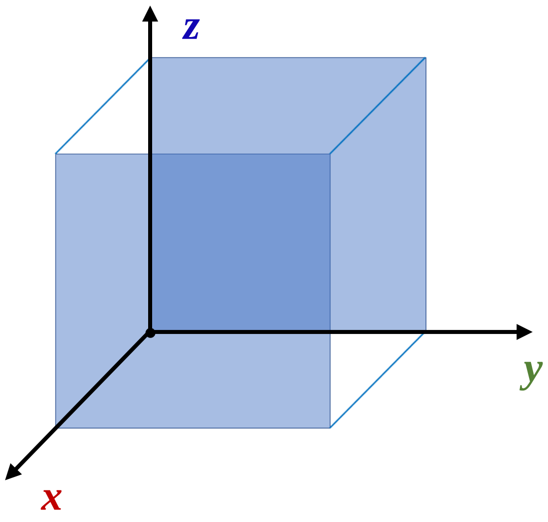


$$\begin{bmatrix} u & v & w \\ h_1 & k_1 & l_1 \\ h_2 & k_2 & l_2 \end{bmatrix} = 0$$

$$\therefore \quad u = (k_1 l_2 - k_2 l_1)$$

$$v = -(h_1 l_2 - l_1 h_2)$$

$$w = (h_1 k_2 - h_2 k_1)$$



Lattice plane parallel to the two directions

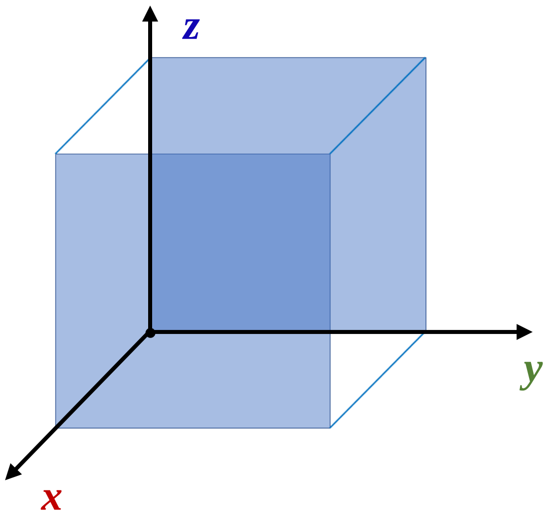
(hkl) $\qquad$ $[u_1 v_1 w_1]$ and $[u_2 v_2 w_2]$

$$\therefore \begin{vmatrix} h & k & l \\ u_1 & v_1 & w_1 \\ u_2 & v_2 & w_2 \end{vmatrix} = 0$$

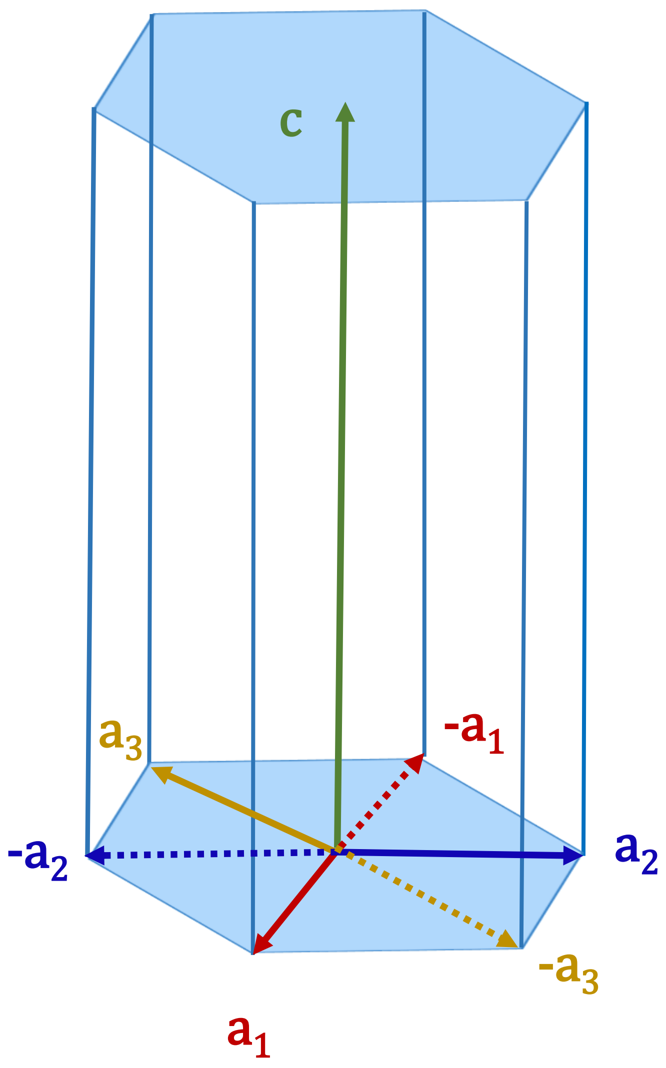
$$\therefore h = (v_1 w_2 - v_2 w_1)$$

$$k = -(u_1 w_2 - u_2 w_1)$$

$$l = (u_1 v_2 - u_2 v_1)$$



Miller-Bravais indices for hexagonal system

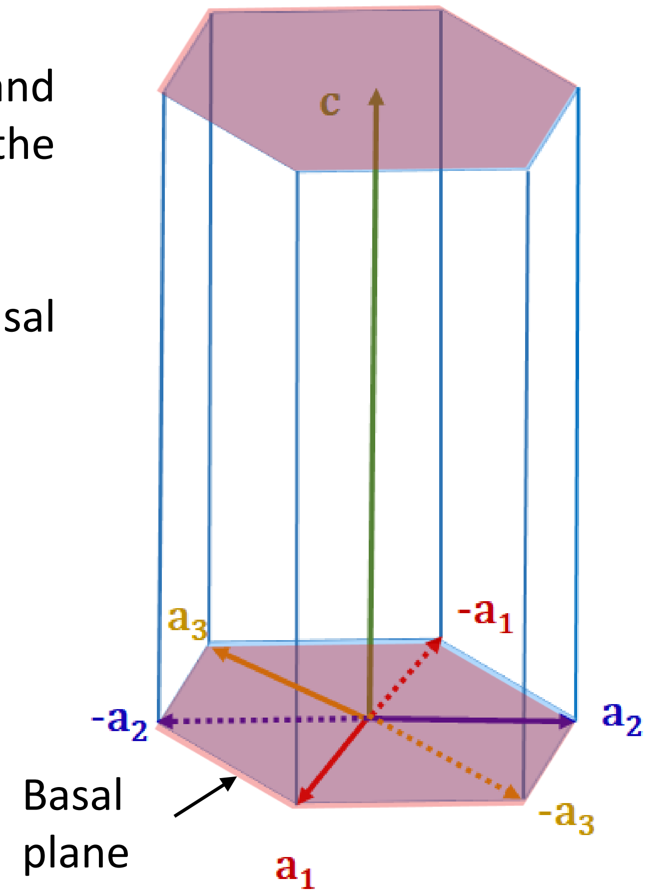


h	k	i	l
↓	↓	↓	↓
a_1	a_2	a_3	c

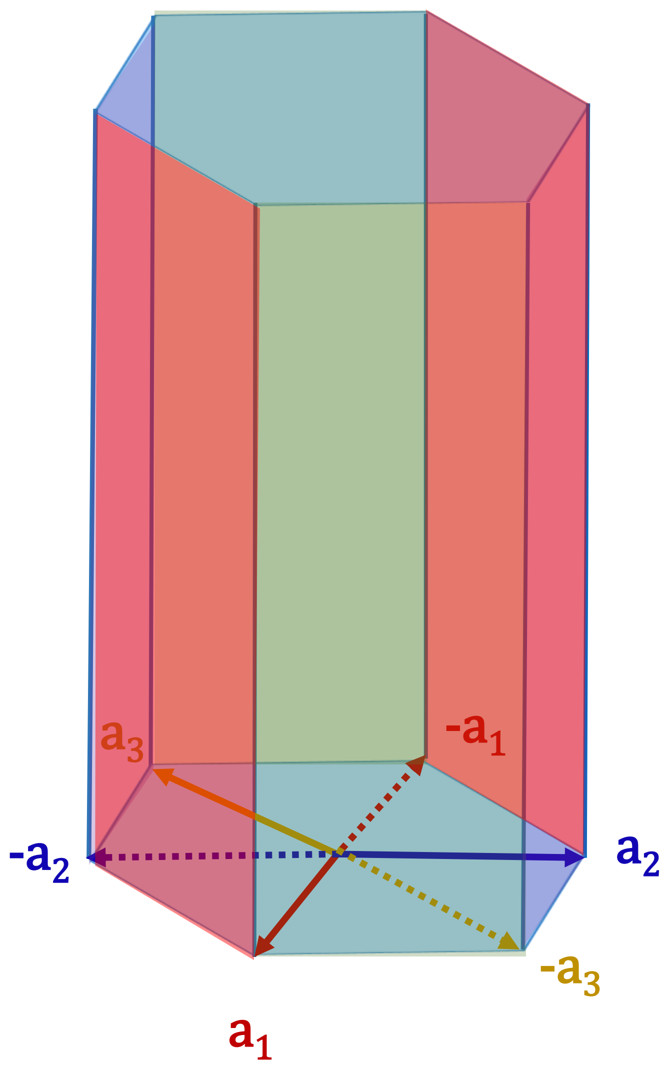
$$i = -(h + k)$$

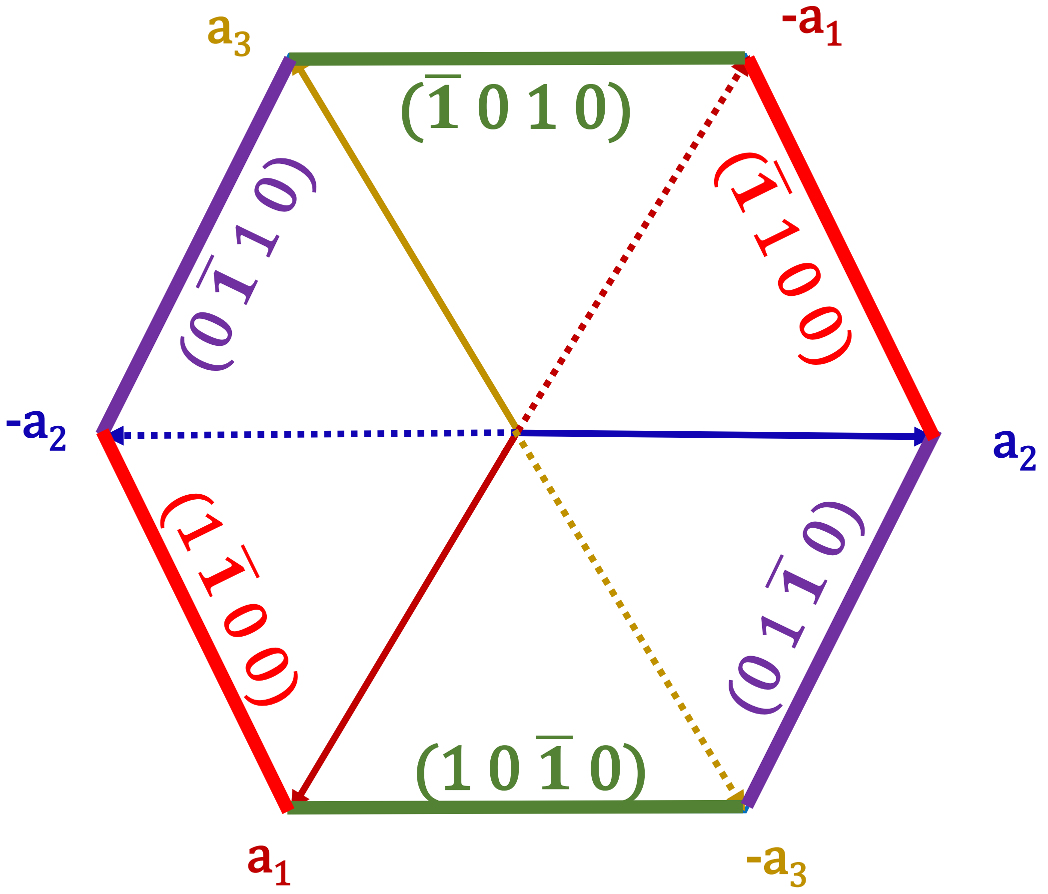
- a_1, a_2 and a_3 are three close-packed directions and are coplanar, lying on the basal plane of the crystal. These axes are at 120° w.r.t each other.
- Fourth axis, c-axis, is perpendicular to the basal plane.
- a_3-axis is the redundant axis.

Intercepts	∞	∞	∞	1
Reciprocals	$\frac{1}{\infty}$	$\frac{1}{\infty}$	$\frac{1}{\infty}$	$\frac{1}{1}$
Plane	(0001)			



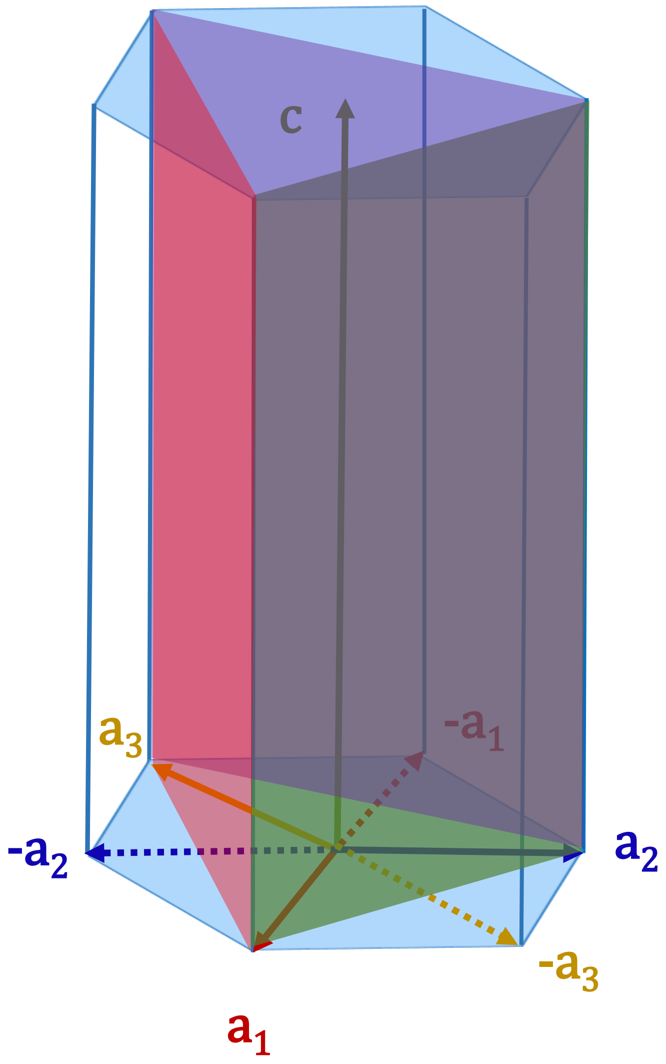
Prismatic planes : *Planes || to the c-axis*

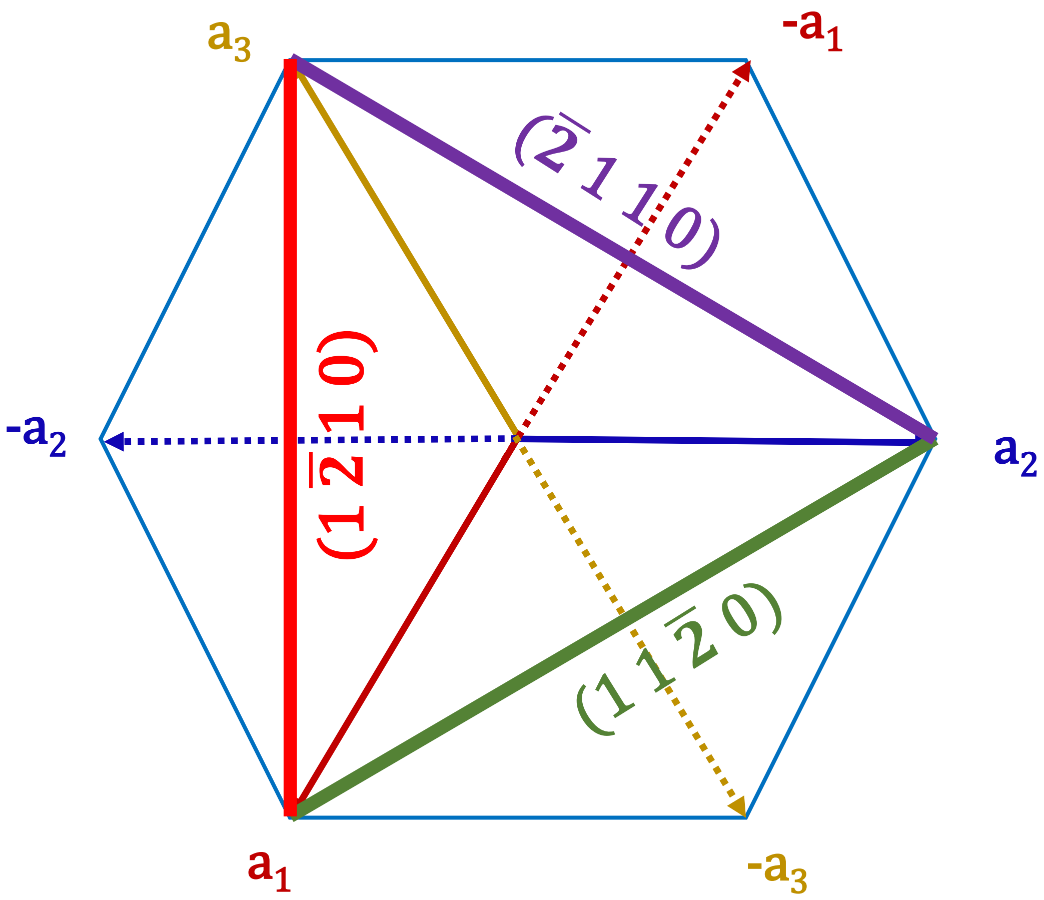


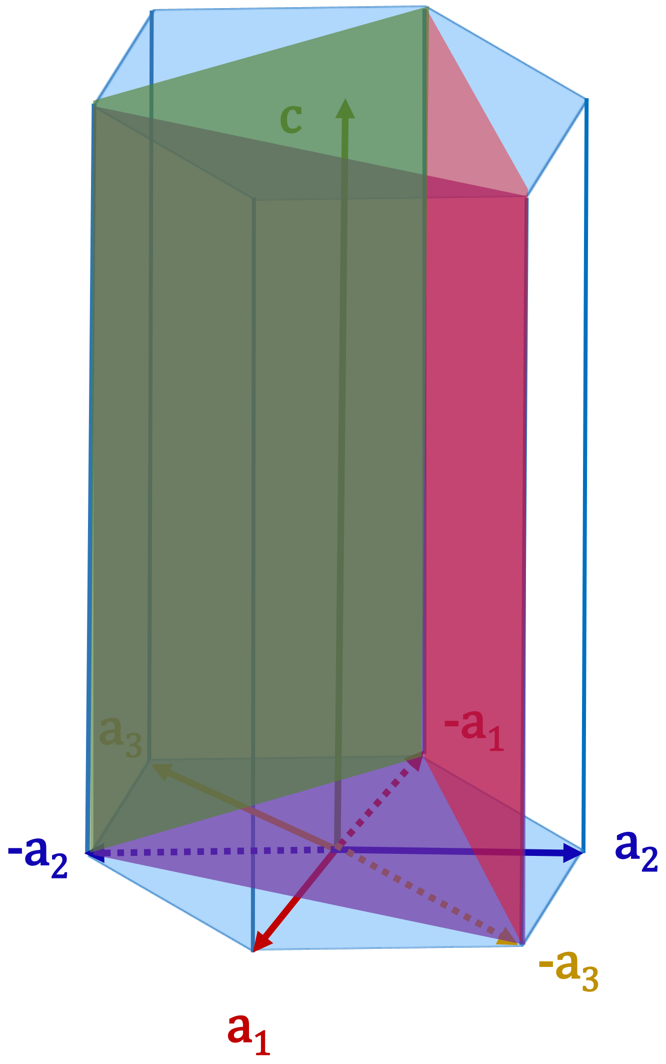


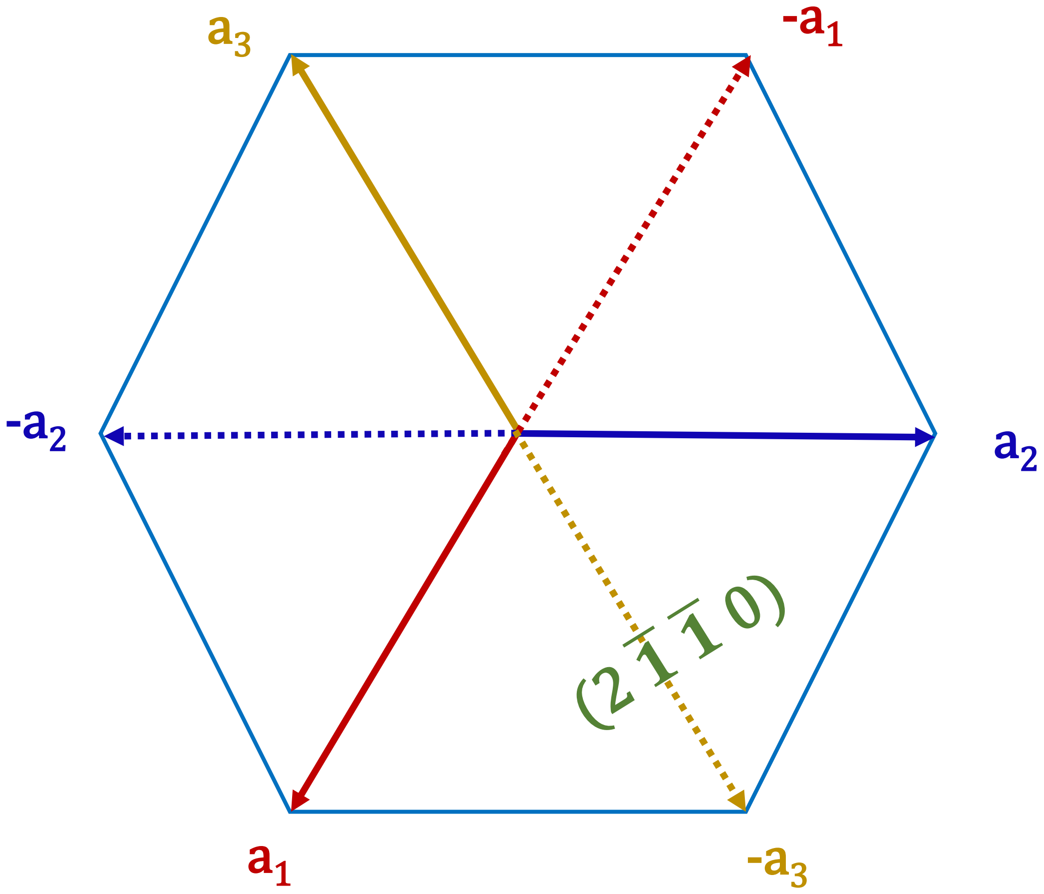
- The equivalent planes, (1 0 0), (0 1 0), $(1\ \bar{1}\ 0)$ defined by Miller indices, got transformed to $(1\ 0\ \bar{1}\ 0)$, $(0\ 1\ \bar{1}\ 0)$ and $(1\ \bar{1}\ 0\ 0)$ defined by Miller-Bravais indices.
- These have the same set of indices, and belong to the same family of planes: $\{1\ \bar{1}\ 0\ 0\}$

Prismatic planes : *Planes || to the c-axis*

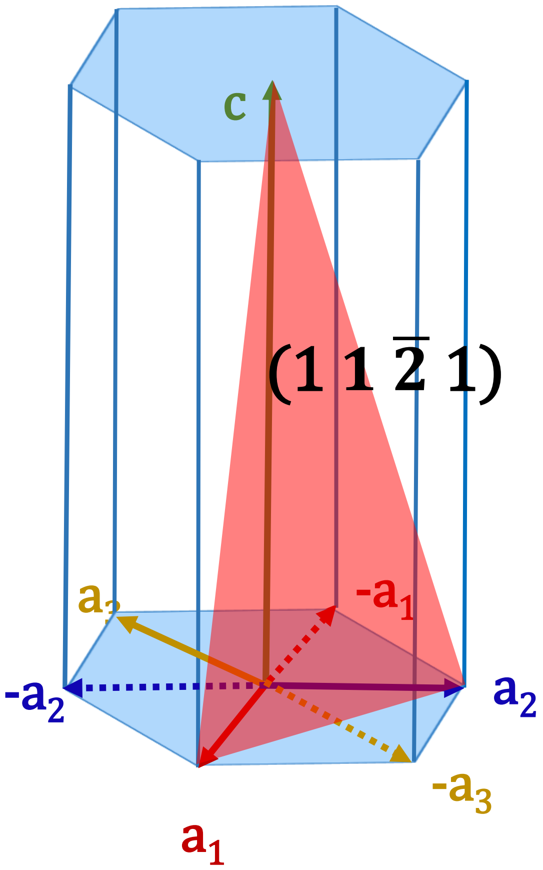


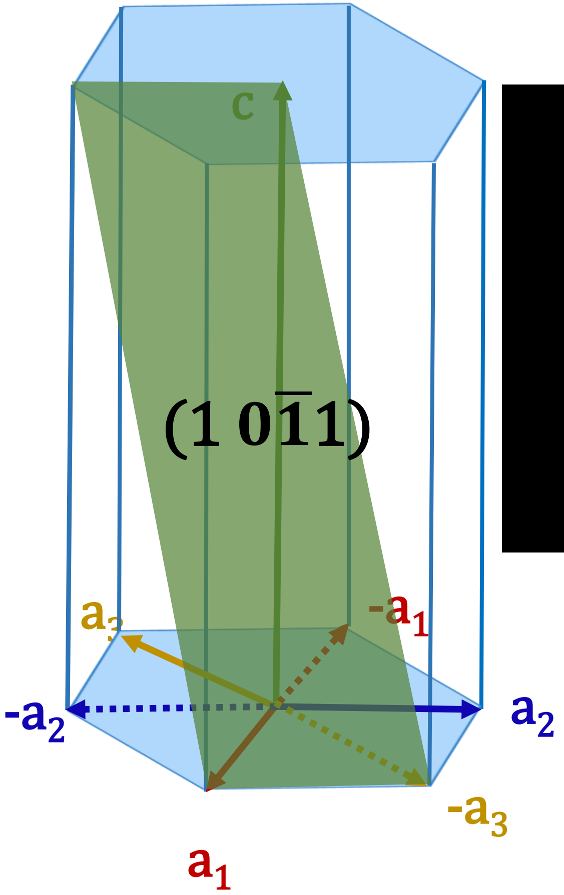


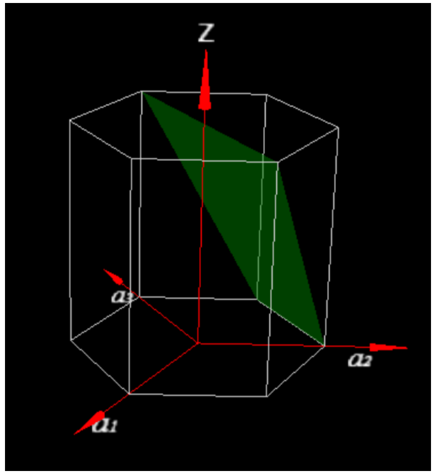

c
a3
-a1
-a2
a2
-a3
a1

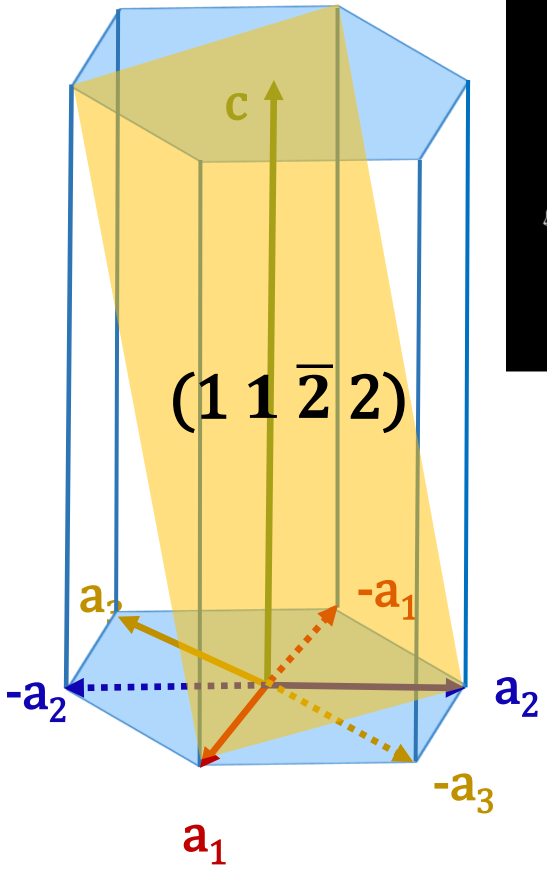

a3
-a1
-a2
a2
(2 1̄ 1̄ 0)
a1
-a3

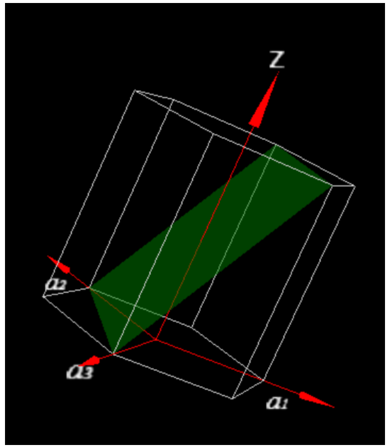
Pyramidal planes : ***Planes which have finite intercepts with the c-axis***









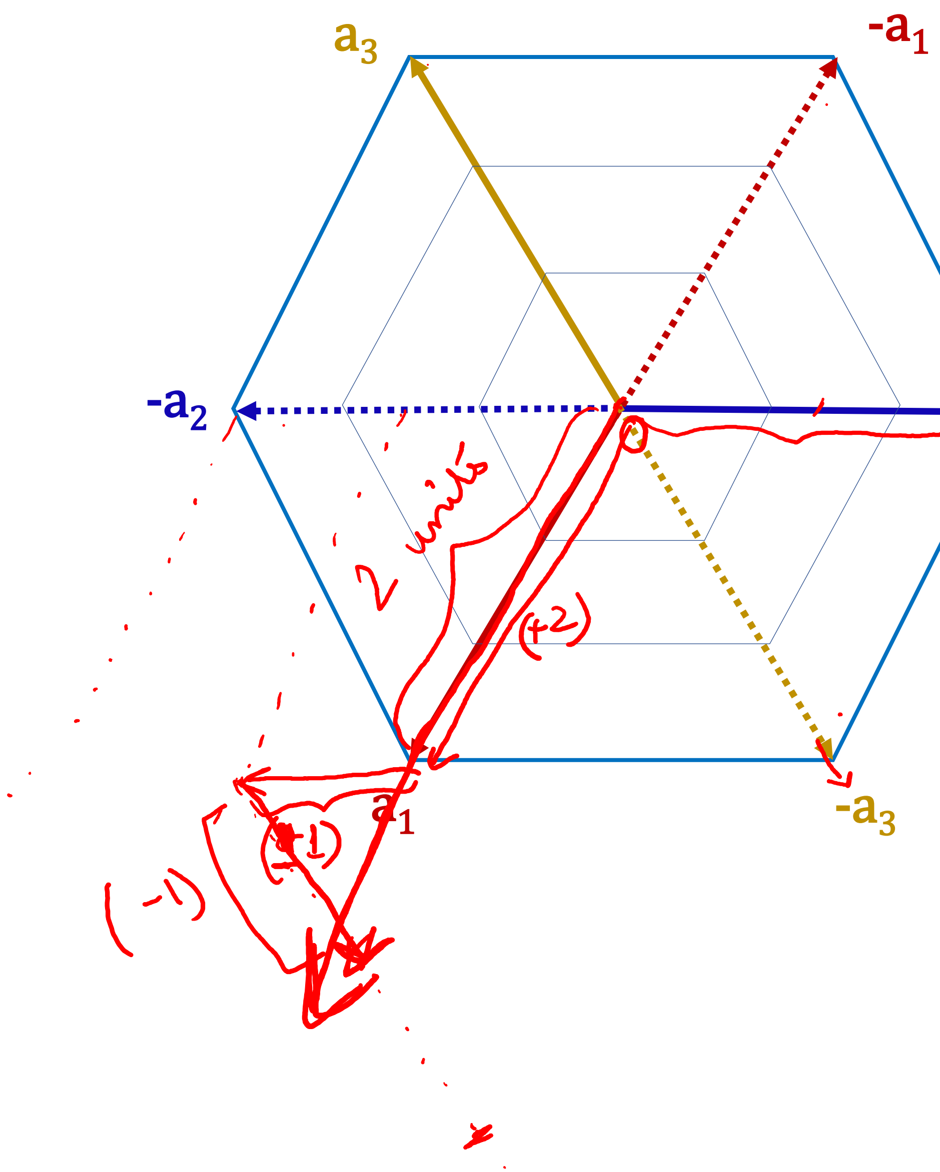


Miller-Bravais directions: *Axis directions*

$a_1 \Rightarrow [1\,0\,0\,0]$ ✗

a_1

$2\,\bar{1}\,\bar{1}\,0$



Highest integer $\Rightarrow 2$

(i) $a_1 \rightarrow (+2)$ units

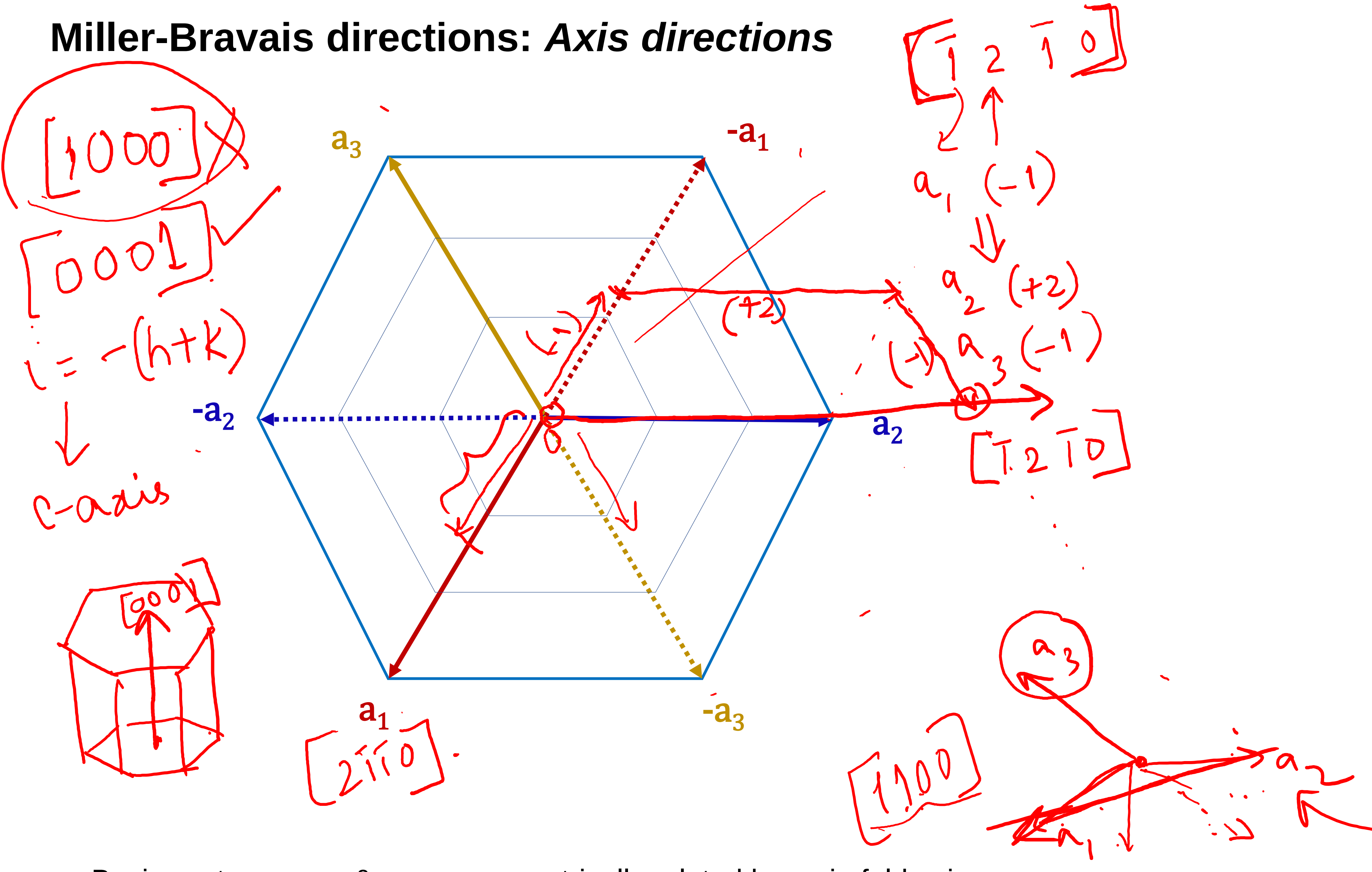
$\Downarrow$

$a_2 \rightarrow (-1)$ units

$\Downarrow$

(f) $a_3 \rightarrow (-1)$ units

Miller-Bravais directions: *Axis directions*



$2\,\bar{1}\,\bar{1}\,0$

$\bar{1}\,2\,\bar{1}\,0$

$\bar{1}\,\bar{1}\,2\,0$

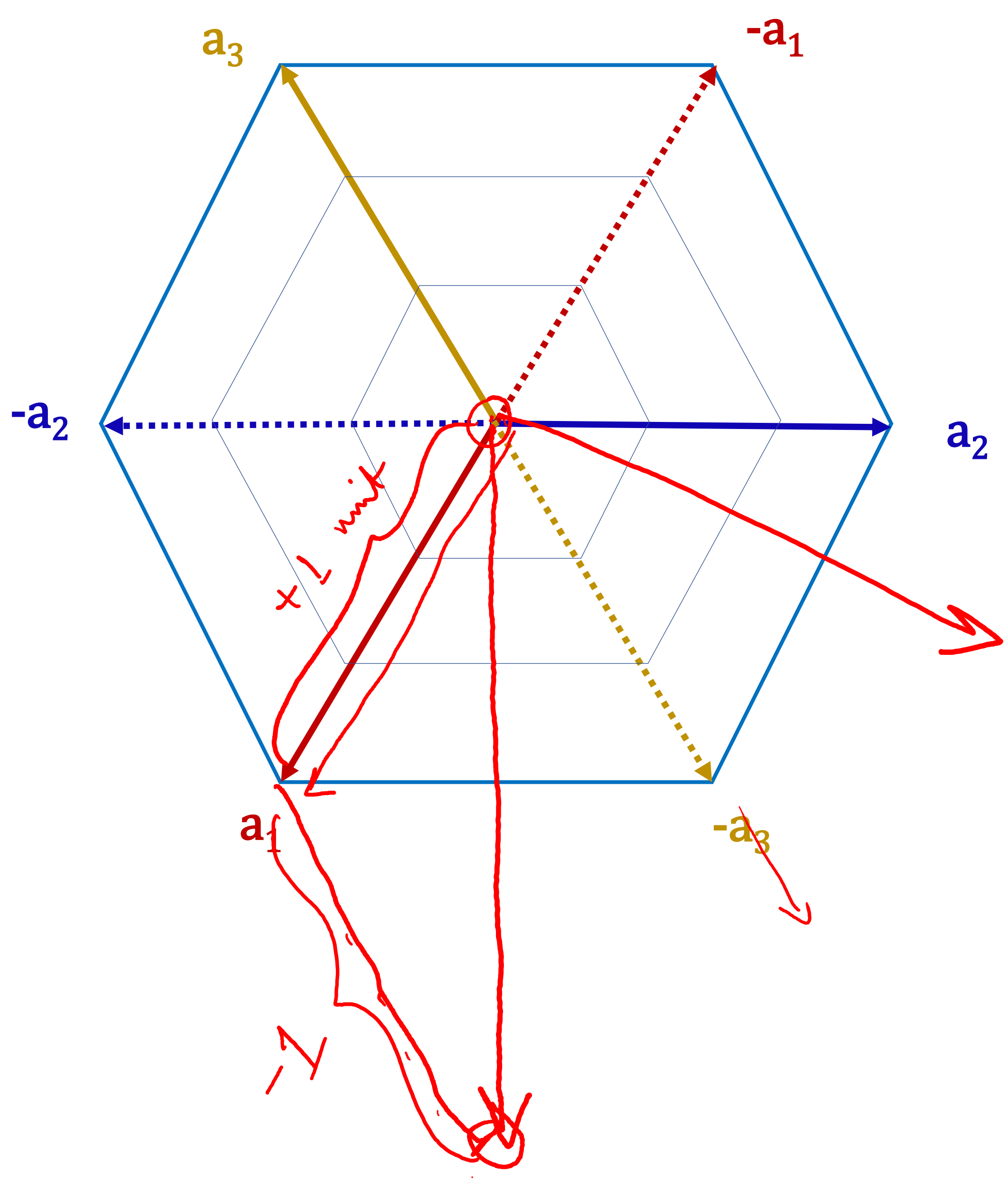
$1\,1\,\bar{2}\,0$

$\bar{2}\,1\,1\,0$

$1\,\bar{2}\,1\,0$

- Basis vectors a_1, a_2 & a_3 are symmetrically related by a six-fold axis.
- The 3rd index is redundant and is included to bring out the equality between equivalent directions (like in the case of planes).

Miller-Bravais directions : *Diagonal directions*



$1\ 0\ \bar{1}\ 0$

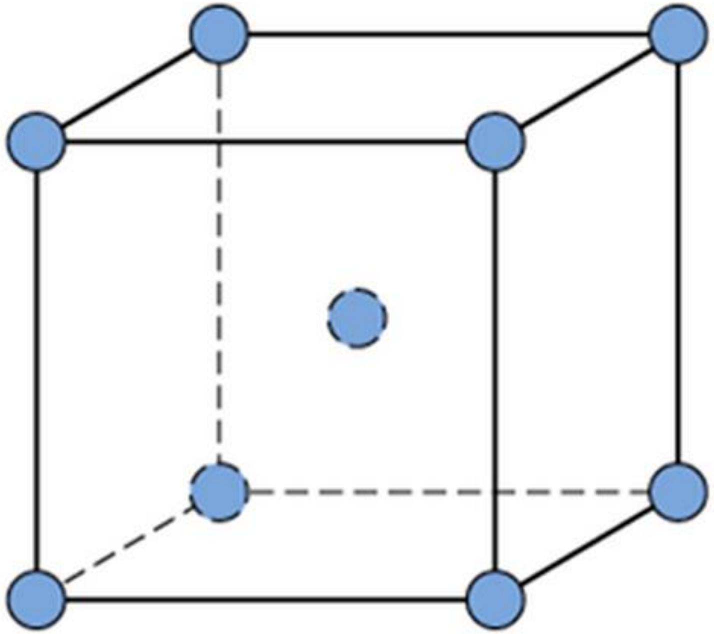
$0\ 1\ \bar{1}\ 0$

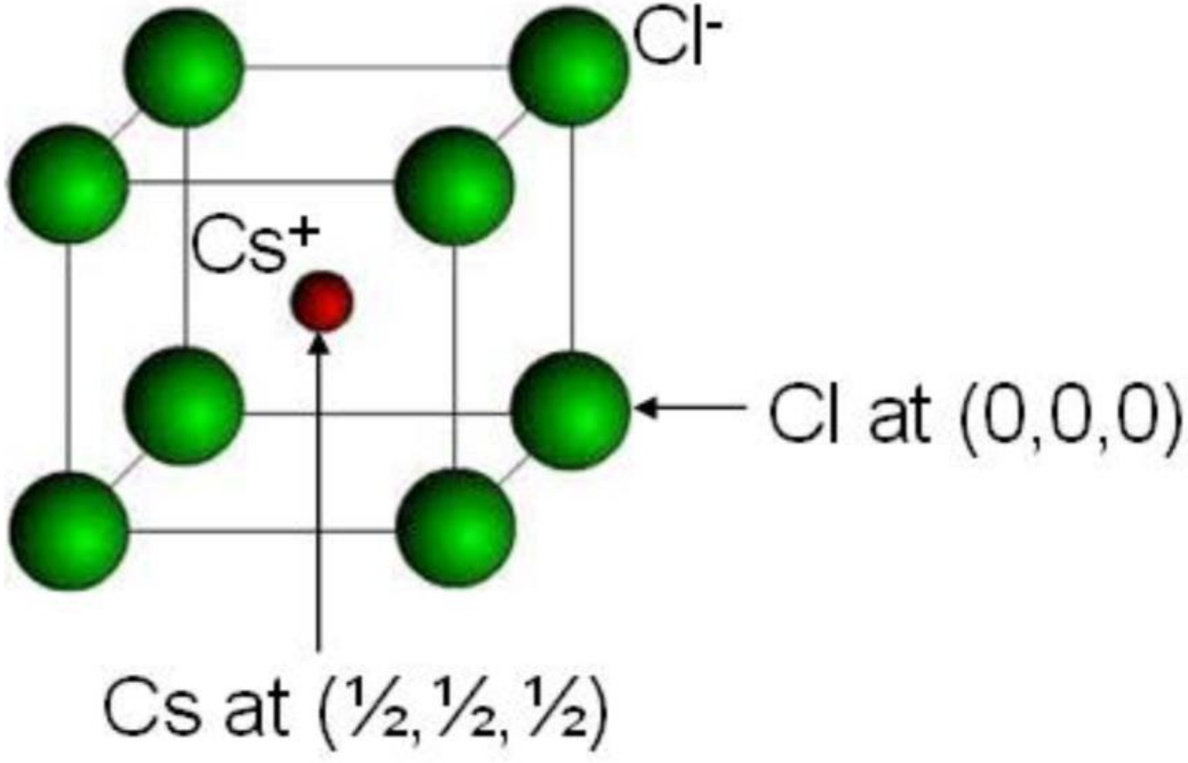
$\bar{1}\ 1\ 0\ 0$

$\bar{1}\ 0\ 1\ 0$

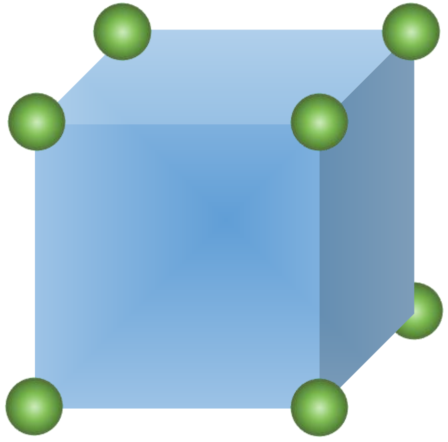
$0\ \bar{1}\ 1\ 0$

$1\ \bar{1}\ 0\ 0$





	Iron (Fe)	CsCl
Motif	1	2
Lattice type	Non-primitive	Primitive
Crystal system	Cubic	Cubic
Bravais lattice	Body centered cubic	Simple cubic



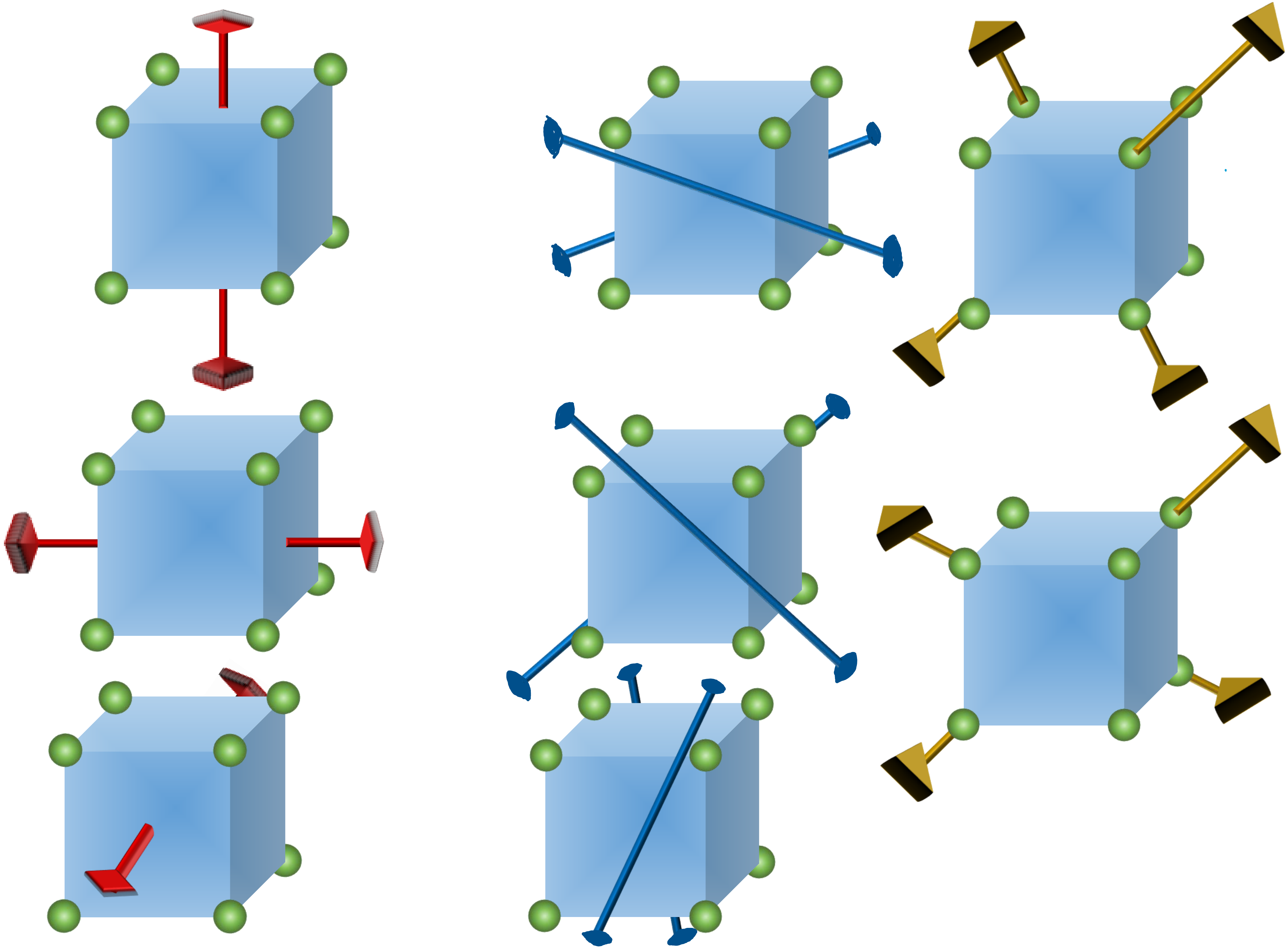
Point symmetry =1

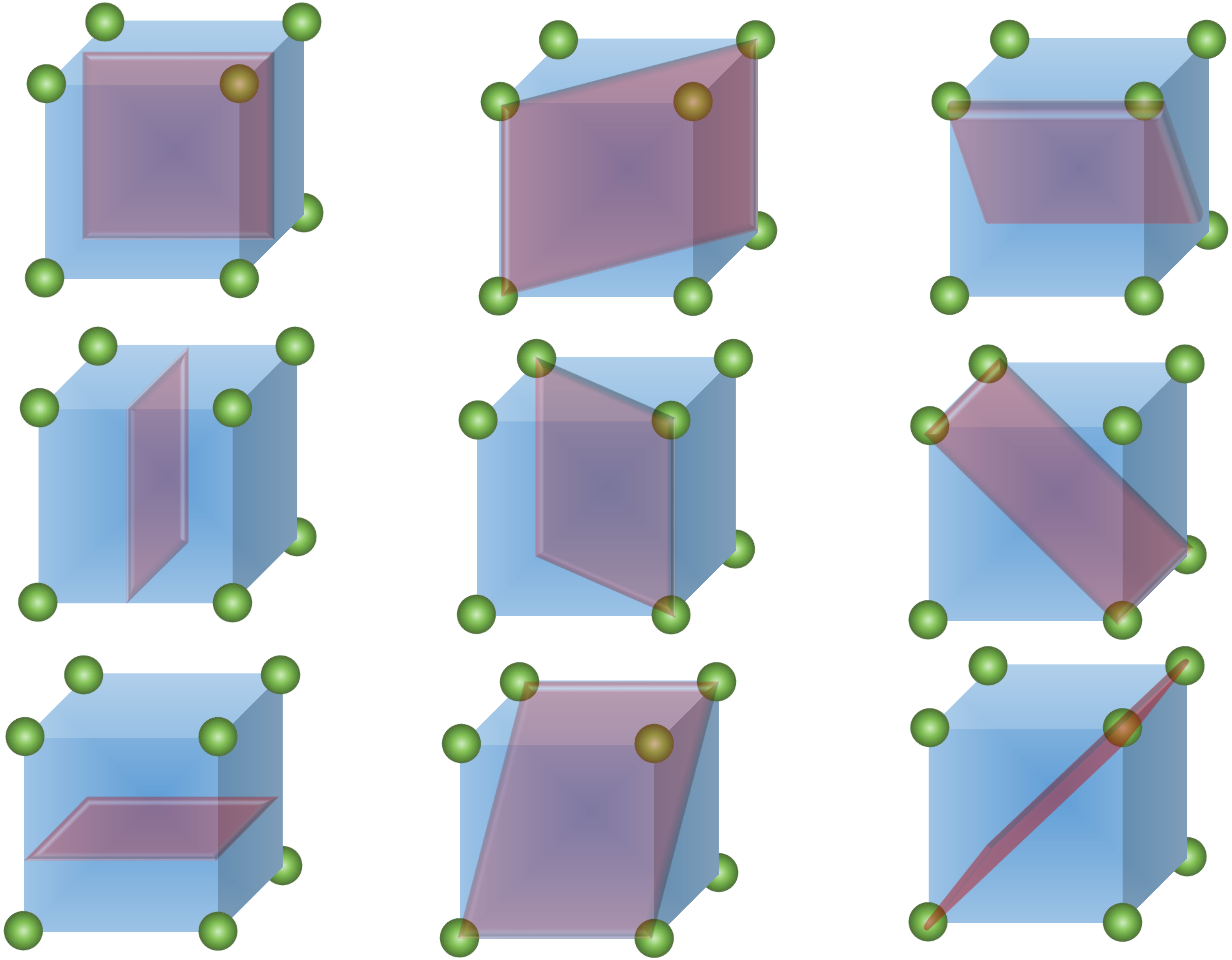
Line of symmetry:

4-fold: 3

2-fold: 6

3-fold: 4

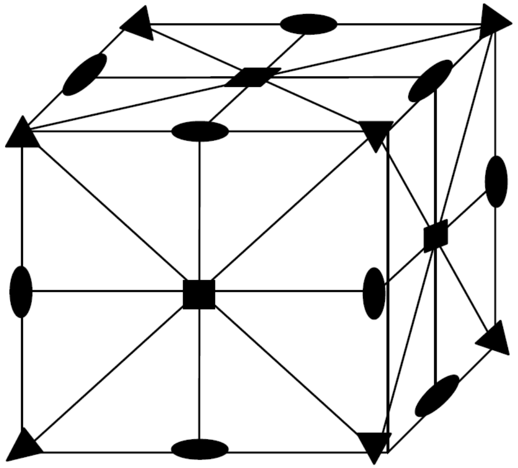




Plane of symmetry:

Mirror plane: 9

Total symmetry in a cube: 1 + 13 + 9 = 23



- What is the difference between crystal structure and crystal system?

- Do non-crystalline materials exhibit the allotropy/polymorphic phenomenon?