MILLER INDICES

- PLANES
- DIRECTIONS

- Lattices
- Crystals

Part of

MATERIALS SCIENCE
&
ENGINEERING

A Learner's Guide

AN INTRODUCTORY E-BOOK

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From the law of rational indices developed by French Physicist and mineralogist
Abbé René Just Haüy
and popularized by
William Hallowes Miller

- Miller indices are used to specify directions and planes.
- These directions and planes could be in lattices or in crystals.
- *(It should be mentioned at the outset that special care should be given to see if the indices are in a lattice or a crystal).*
- The number of indices will match with the dimension of the lattice or the crystal: in 1D there will be 1 index and 2D there will be two indices etc.
- Some aspects of Miller indices, especially those for planes, are not intuitively understood and hence some time has to be spent to familiarize oneself with the notation.

Note: both directions and planes are imaginary constructs

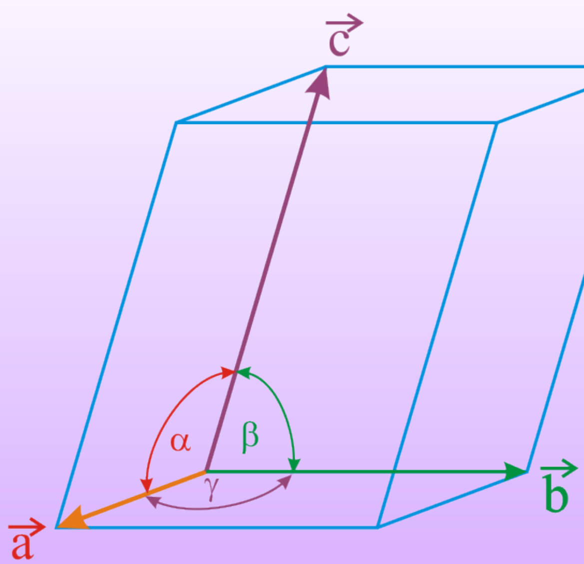
Miller indices for DIRECTIONS

A vector **r** passing from the origin to a lattice point can be written as: $\mathbf{r} = r_1\,\mathbf{a} + r_2\,\mathbf{b} + r_3\,\mathbf{c}$

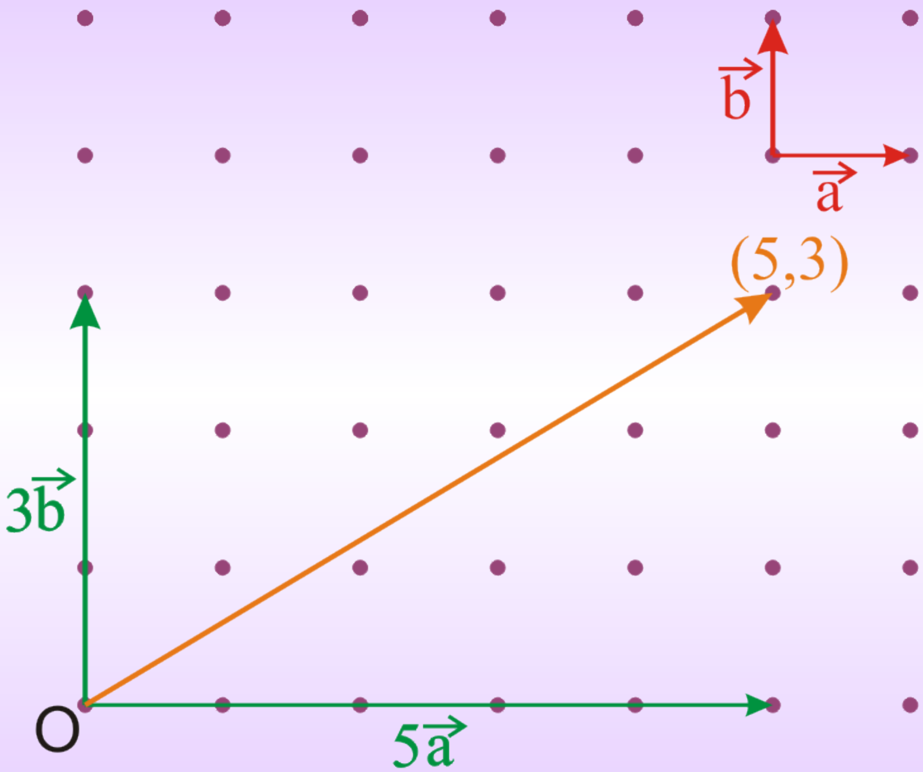
$$r = r_1\,\vec{a} + r_2\,\vec{b} + r_3\,\vec{c}$$

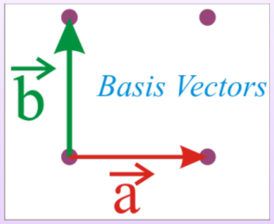
Where, **a**, **b**, **c** → basic vectors

- Basis vectors are unit lattice translation vectors which define the coordinate axis *(as in the figure below)*.
- *Note their length is not 1 unit! (like for the basis vectors of a coordinate axis).*



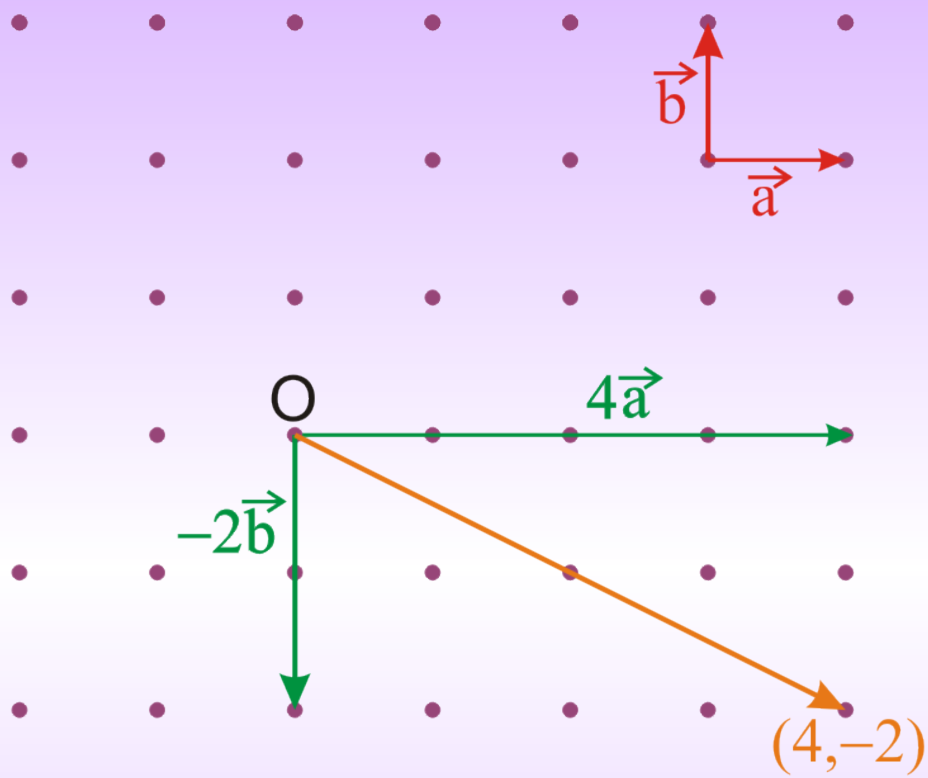
Miller Indices for directions in 2D





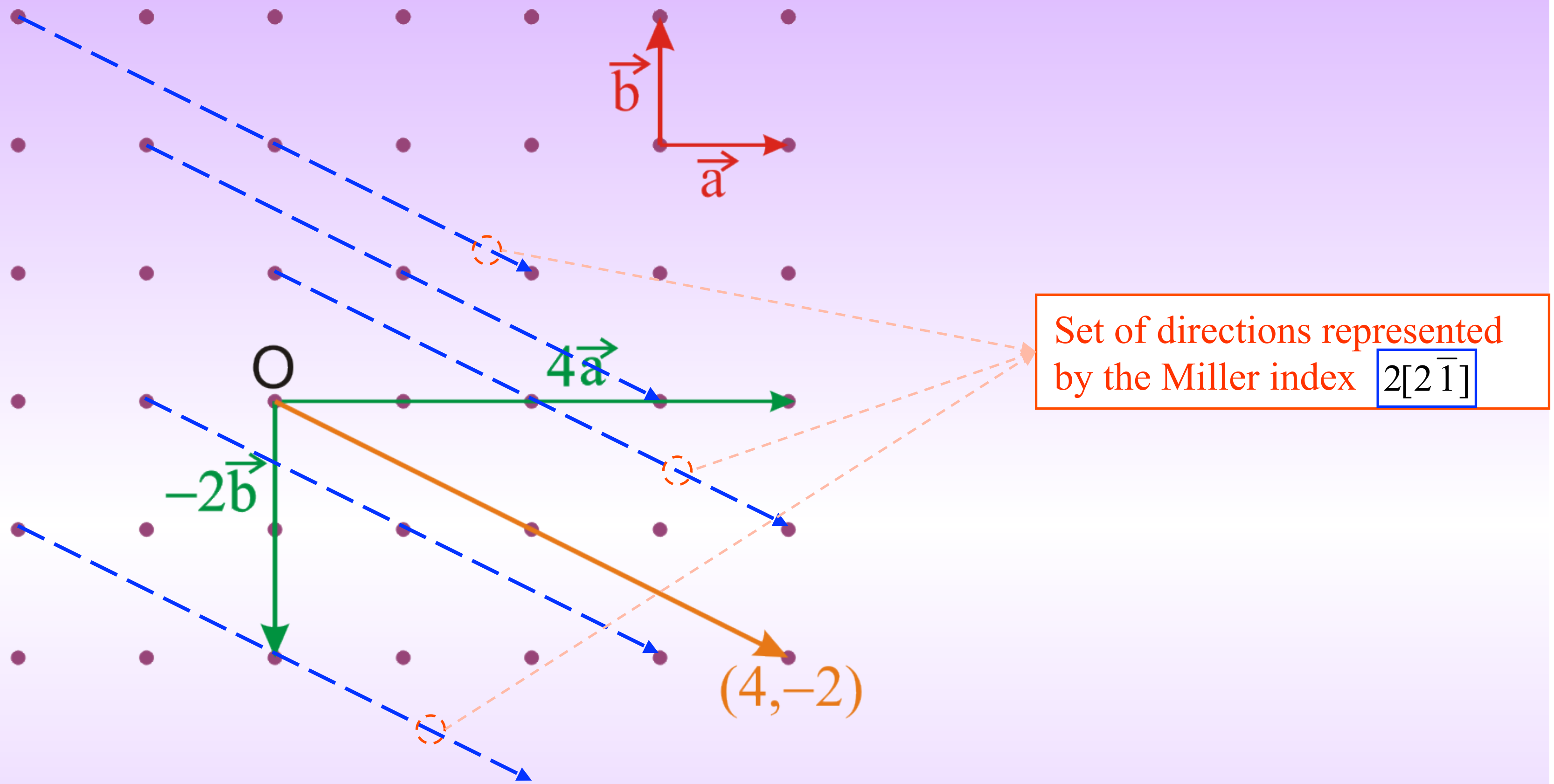
Miller indices → [53]

Another 2D example



$Miller\ Indices\ for\ the\ direction\ with\ magnitude \rightarrow 2[2\,\bar{1}]$

$Miller\ Indices\ for\ just\ the\ direction \rightarrow [2\,\bar{1}]$



Miller Indices → $2[2\bar{1}]$

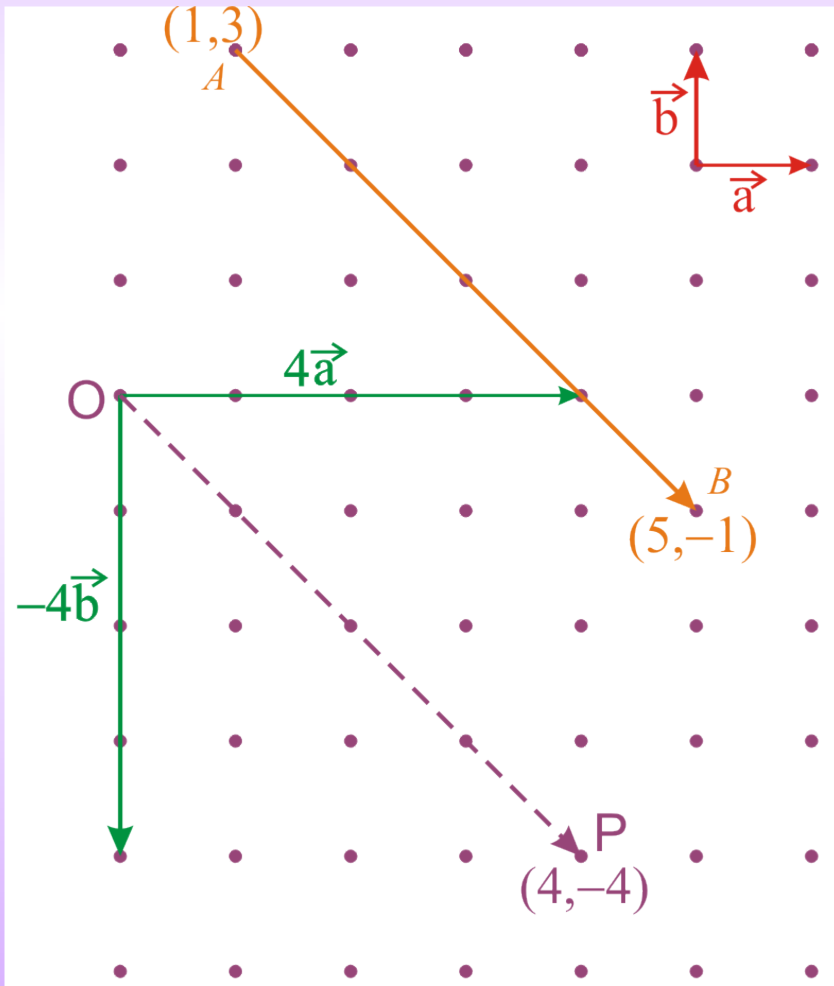
The index represents a set of all such parallel vectors *(and not just one vector)*

(Note: 'usually' (actually always for now!)

originating at a lattice point and ending at a lattice point)

How to find the Miller Indices for an arbitrary direction? → Procedure

- Consider the example below
- Subtract the coordinates of the end point from the starting point of the vector denoting the direction → If the starting point is A(1,3) and the final point is B(5,-1) → the difference would be (4, -4)



- Enclose in square brackets, remove comma and write negative numbers with a bar → $[4\,\bar{4}]$
- Factor out the common factor → $4[1\,\bar{1}]$

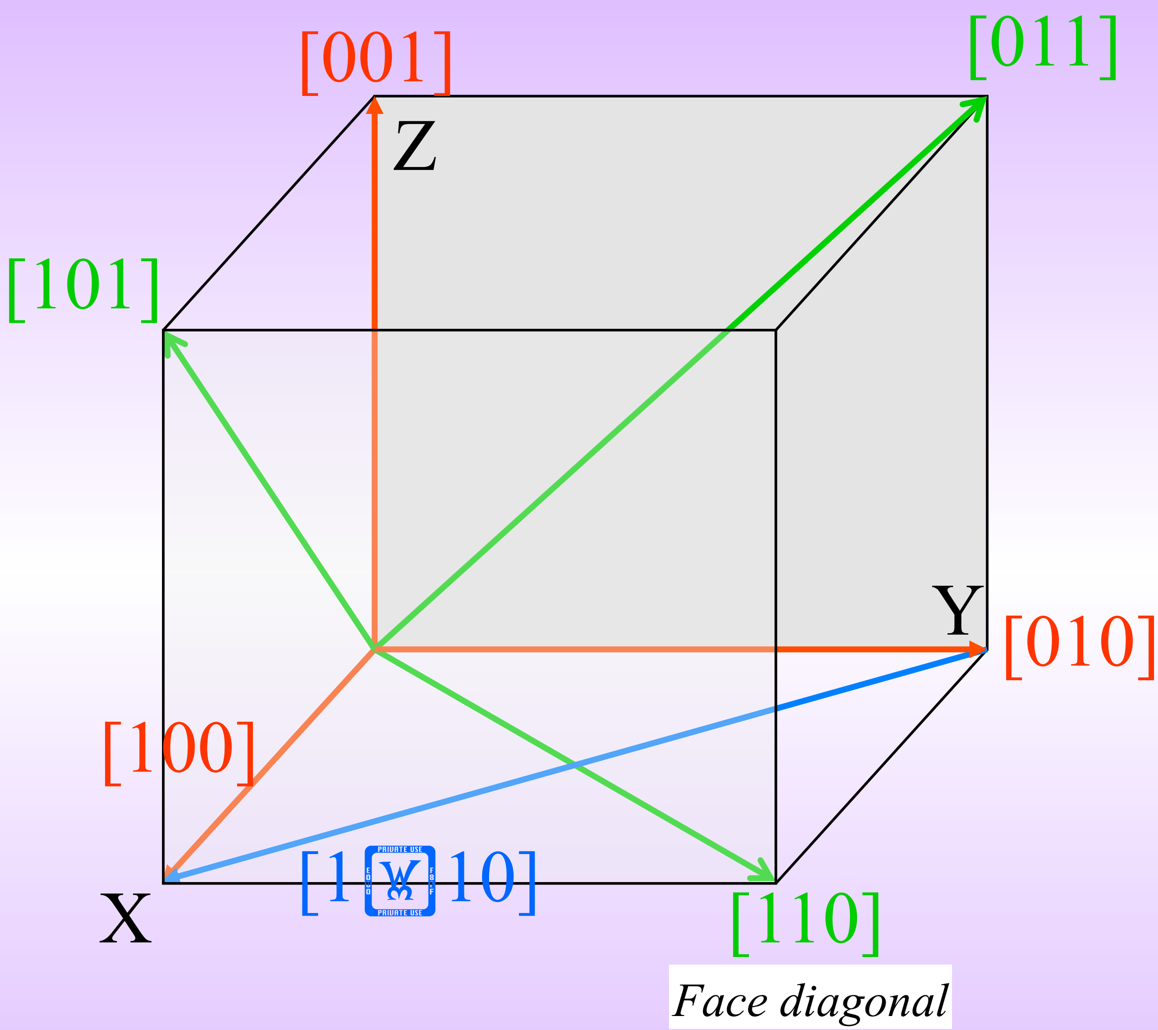
- If we are worried about the direction and magnitude then we write → $4[1\,\bar{1}]$
- If we consider only the direction then we write → $[1\,\bar{1}]$
- Needless to say the first vector is 4 times in length
- The magnitude of the vector $[1\,\bar{1}] = |[1\,\bar{1}]|$ is $\sqrt{(1)^2 + (-1)^2} = \sqrt{2}$

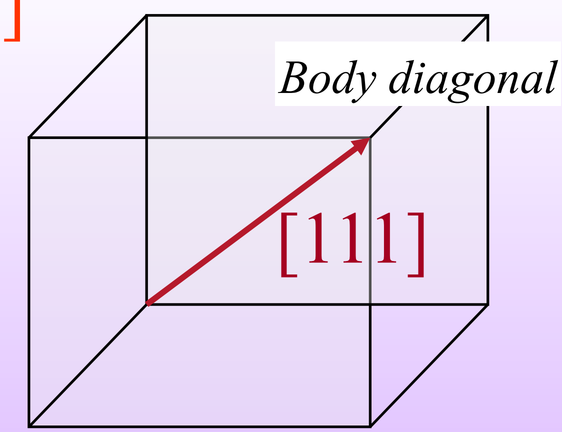
Further points

- General Miller indices for a direction in 3D is written as [u v w]
- The length of the vector represented by the Miller indices is: $\sqrt{u^2 + v^2 + w^2}$

Important directions in 3D represented by Miller Indices (cubic lattice)

Memorize these





Procedure as before:

- (Coordinates of the final point - coordinates of the initial point)
- Reduce to smallest integer values

The concept of a family of directions

- A set of directions related by symmetry operations of the lattice or the crystal is called a family of directions
- A family of directions is represented (Miller Index notation) as: <u v w>
- Hence one has to ask two questions before deciding on the list of the members of a family:
  1➢ *Is one considering the lattice or the crystal?*
  2➢ *What is the crystal system one is talking about*
  (and what are its symmetries; i.e. point group)?

Miller indices for a direction in a lattice versus a crystal

- We have seen in the chapter on geometry of crystals that crystal can have symmetry equal to or lower than that of the lattice.
- If the symmetry of the crystal is lower than that of the lattice then two members belonging to the same family in a lattice need not belong to the same family in a crystal → this is because *crystals can have lower symmetry than a lattice* (examples which will taken up soon will explain this point).

Family of directions

Examples

Let us consider a square lattice:

- [10] and [01] belong to the same family → related by a 4-fold rotation
- [11] and $[\bar{1}1]$ belong to the same family → related by a 4-fold rotation
- [01] and $[0\bar{1}]$ belong to the same family → related by a 2-fold rotation

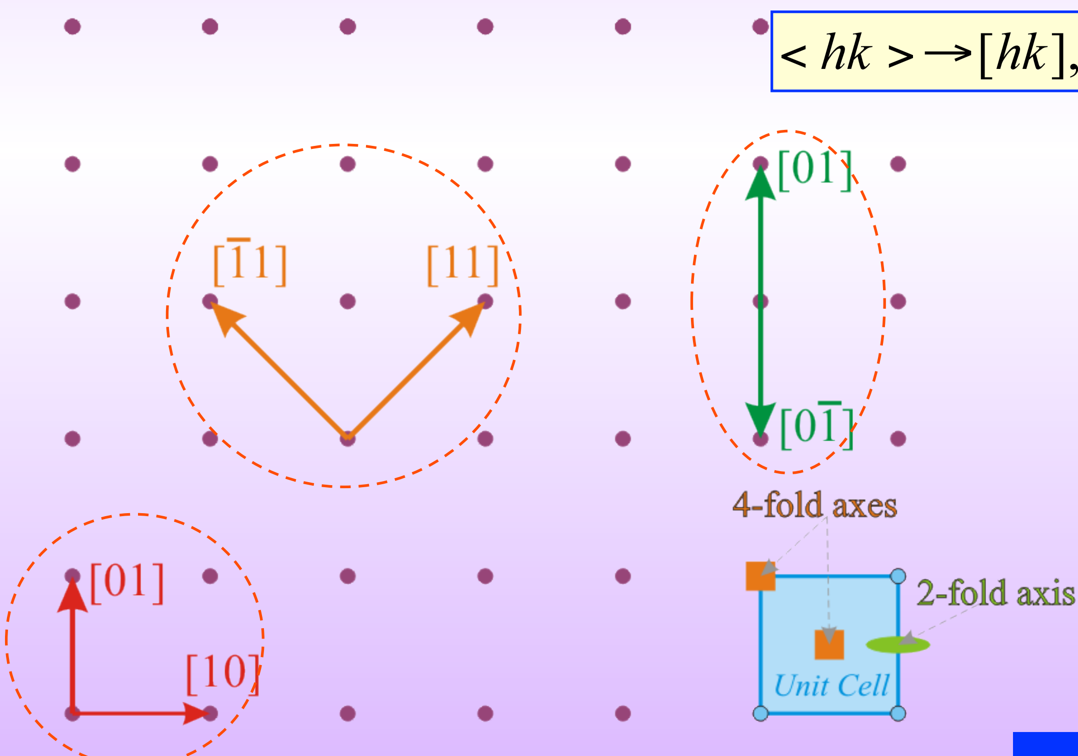
(or double action of 4-fold)

Writing down all the members of the family

$$<hk> \rightarrow [hk],[\bar{h}k],[h\bar{k}],[\bar{h}\,\bar{k}],[kh],[\bar{k}h],[k\bar{h}],[\bar{k}\,\bar{h}]$$

$$<10> \rightarrow [10],[01],[\bar{1}0],[0\bar{1}]$$

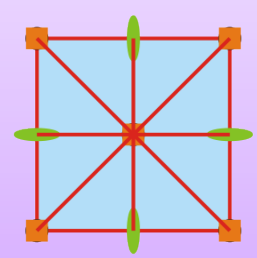
$$<11> \rightarrow [11],[\bar{1}1],[1\bar{1}],[\bar{1}\bar{1}]$$



Essentially the 1st and 2nd index can be interchanged and be made negative (due to high symmetry)

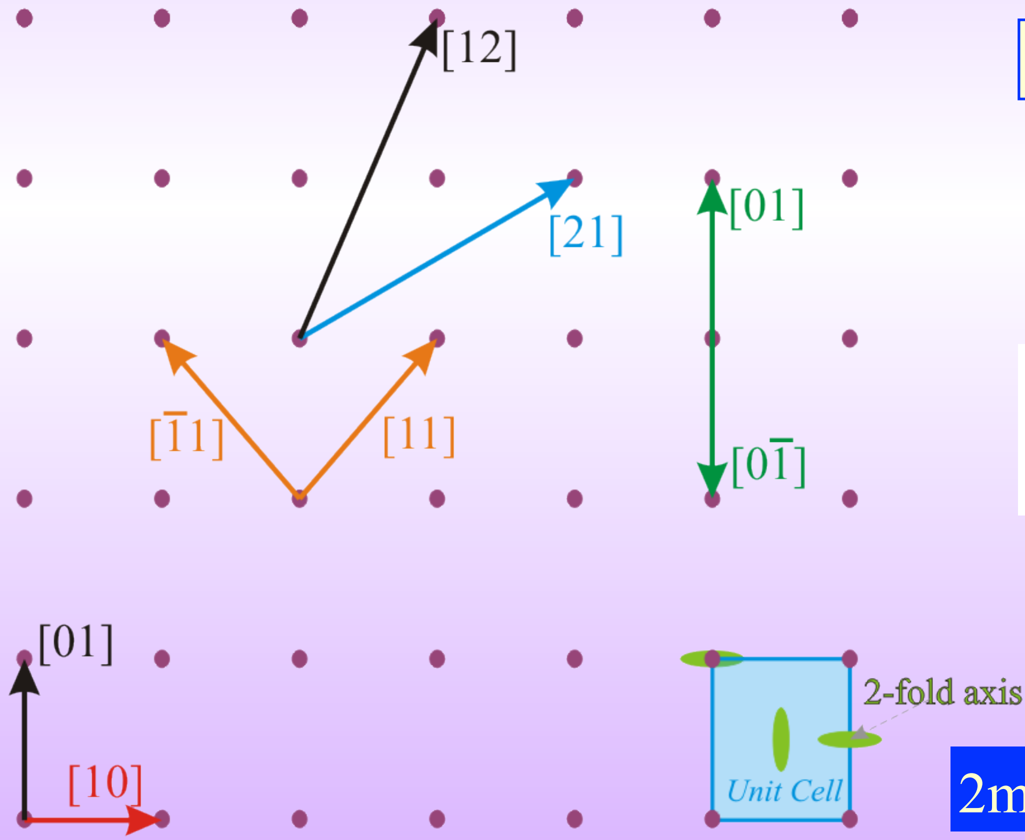
For sake of clarity all symmetry operators have not been marked

4mm



Let us consider a Rectangle lattice:

- [10] and [01] do **NOT** belong to the same family
- [11] and $[\bar{1}1]$ belong to the same family → related by a mirror
- [01] and $[0\bar{1}]$ belong to the same family → related by a 2-fold rotation
- [21] and [12] do **NOT** belong to the same family



For sake of clarity all symmetry axes have not been marked

Writing down all the members of the family

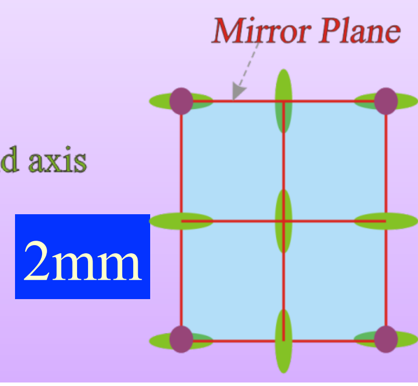
$$< hk > \rightarrow [hk],[\bar{h}k],[h\bar{k}],[\bar{h}\,\bar{k}]$$

$$< 10 > \rightarrow [10],[\bar{1}0]$$

$$< 11 > \rightarrow [11],[\bar{1}1],[1\bar{1}],[\bar{1}\bar{1}]$$

$$< 12 > \rightarrow [12],[\bar{1}2],[1\bar{2}],[\overline{12}]$$

*The 1st and 2nd index can **NOT** be interchanged, but can be made negative*



Let us consider a square lattice decorated with a rotated square to give a SQUARE CRYSTAL *(as 4-fold still present)*:

- [10] and [01] belong to the same family → related by a 4-fold
- [11] and $[\bar{1}1]$ belong to the same family → related by a 4-fold
- [01] and $[0\bar{1}]$ belong to the same family → related by a 4-fold (twice)
- [12] and $[\bar{1}2]$ do NOT belong to the same family

Writing down all the members of the family

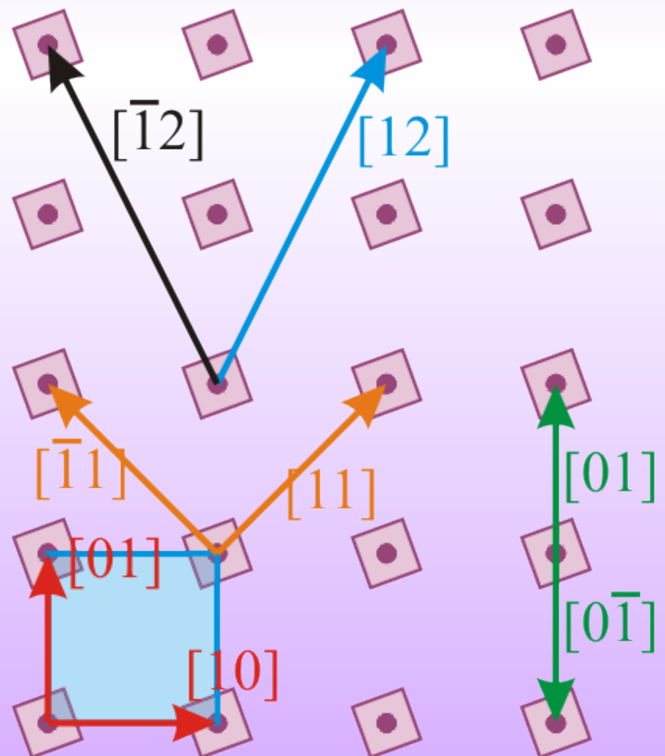
$$< hk > \rightarrow [hk],[\bar{h}\,\bar{k}],[\bar{k}h],[k\bar{h}]$$

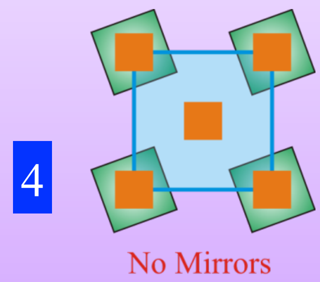
$$< 10 > \rightarrow [10],[\bar{1}0],[01],[0\bar{1}]$$

$$< 11 > \rightarrow [11],[\bar{1}1],[1\bar{1}],[\bar{1}\bar{1}]$$

$$< 12 > \rightarrow [12],[\bar{2}1],[\bar{1}\bar{2}],[2\bar{1}]$$

$$< 21 > \rightarrow [21],[\bar{1}2],[\bar{2}\bar{1}],[1\bar{2}]$$

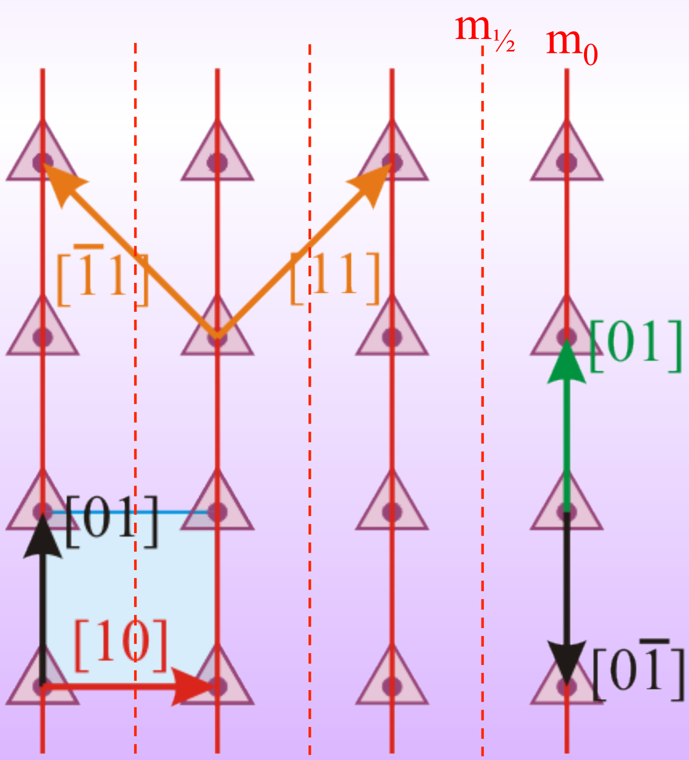


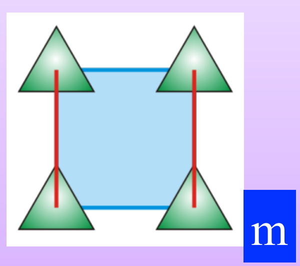


Let us consider a square lattice decorated with a triangle to give a RECTANGLE CRYSTAL:

- [10] and [01] do NOT belong to the same family
  $\rightarrow$ 4-fold rotation destroyed in the crystal
- [11] and $[\bar{1}1]$ belong to the same family $\rightarrow$ related by mirror
- [11] and $[1\bar{1}]$ do NOT belong to the same family
- [01] and $[0\bar{1}]$ do NOT belong to the same family

Thought provoking example





Writing down all the members of the family

$$< hk > \rightarrow [hk], [\bar{h}k]$$

$$< 10 > \rightarrow [10], [\bar{1}0]$$

$$< 01 > \rightarrow [01]$$

$$< 0\bar{1} > \rightarrow [0\bar{1}]$$

$$< 11 > \rightarrow [11], [\bar{1}1]$$

$$< 1\bar{1} > \rightarrow [1\bar{1}], [\bar{1}\bar{1}]$$

Important Note

Hence, all directions related by symmetry (only) form a family

Family of directions

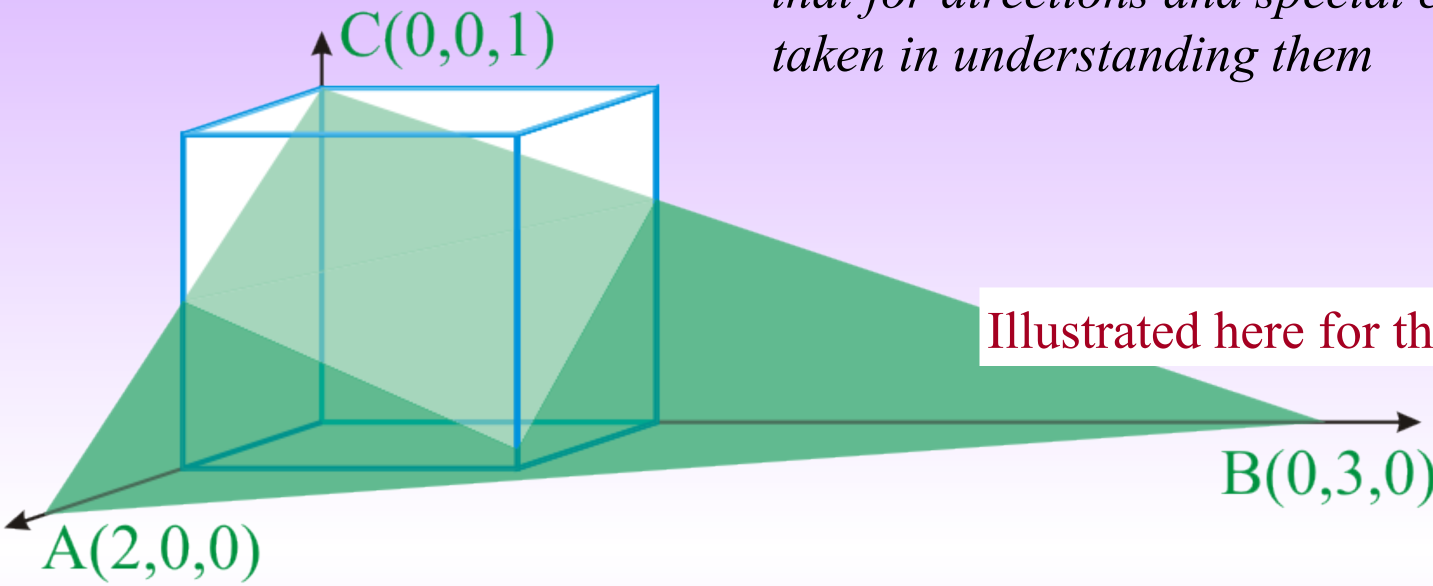
Index	Members in family for **cubic lattices**	Number
<100>	$[100],[\bar{1}00],[010],[0\bar{1}0],[001],[00\bar{1}]$	3 x 2 = 6
<110>	$[110],[\bar{1}10],[1\bar{1}0],[\bar{1}\bar{1}0],[101],[\bar{1}01],[10\bar{1}],[\bar{1}0\bar{1}],[011],[0\bar{1}1],[01\bar{1}],[0\bar{1}\bar{1}]$	6 x 2 = 12
<111>	$[111],[\bar{1}11],[1\bar{1}1],[11\bar{1}],[\bar{1}\bar{1}1],[\bar{1}1\bar{1}],[1\bar{1}\bar{1}],[\bar{1}\bar{1}\bar{1}]$	4 x 2 = 8

the ‘negatives’ (opposite direction)

Symbol	Alternate symbol		
[ ]		→	Particular direction
< >	[[ ]]	→	Family of directions

Miller Indices for PLANES

Miller indices for planes is not as intuitive as that for directions and special care must be taken in understanding them



Illustrated here for the cubic lattice

- ❑ Find intercepts along axes → 2 3 1
- ❑ Take reciprocal → 1/2 1/3 1*
- ❑ Convert to smallest integers in the same ratio → 3 2 6
- ❑ Enclose in parenthesis → (326)

- ➢ Note: (326) does NOT represent one plane but *a* ***set*** *of parallel planes* passing through lattice points.
- ➢ Set of planes should not be confused with a family of planes- which we shall consider next.

* *As we shall see later- reciprocals are taken to avoid infinities in the 'defining indices' of planes*

Funda Check

- Why do need Miller indices (say for planes)?
- Can’t we just use intercepts to designate planes?

Thus we see that Miller indices does the following:

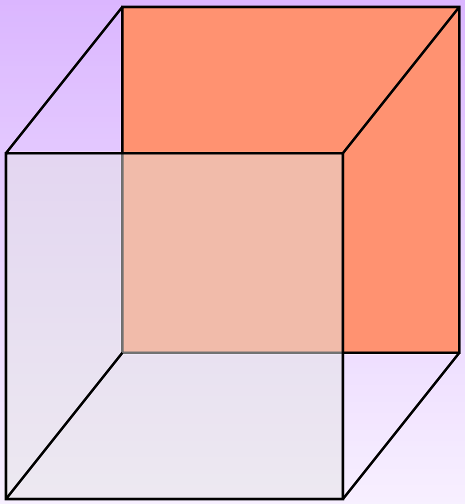
- Avoids infinities in the indices (intercepts of (1, ∞, ∞) becomes (100) index).
- Avoids dimensioned numbers
  - I*nstead we have multiples of lattice parameters along the* ***a, b, c*** *directions (this implies that 1a could be 10.2Å, while 2b could be 8.2Å).*

The concept of a family of planes

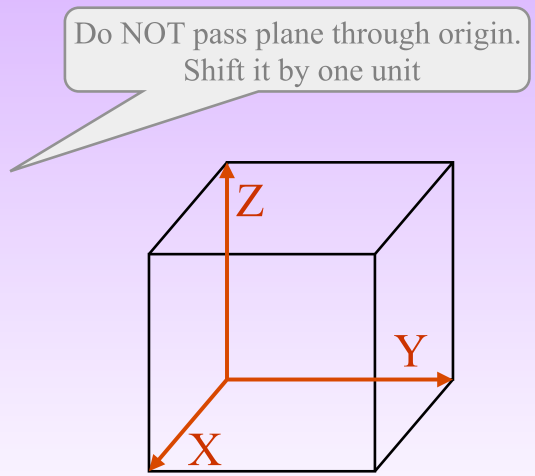
- A set of planes related by symmetry operations of the lattice or the crystal is called a family of planes (the translation symmetry operator is excluded→ the translational symmetry is included in the definition of a plane itself*).
- All the points which one should keep in mind while dealing with directions to get the members of a family, should also be kept in mind when dealing with planes.

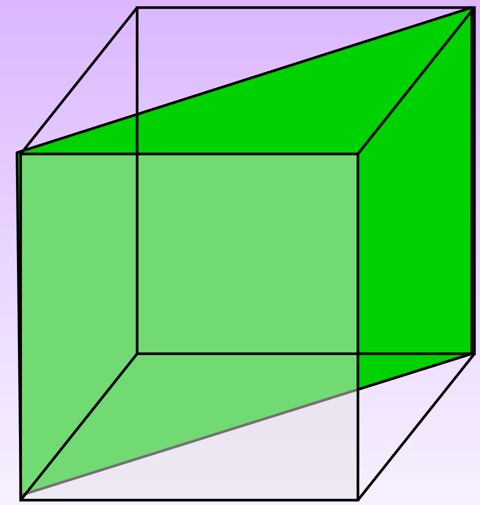
** As the Miller index for a plane line (100) implies a infinite parallel set of planes.*

Cubic lattice



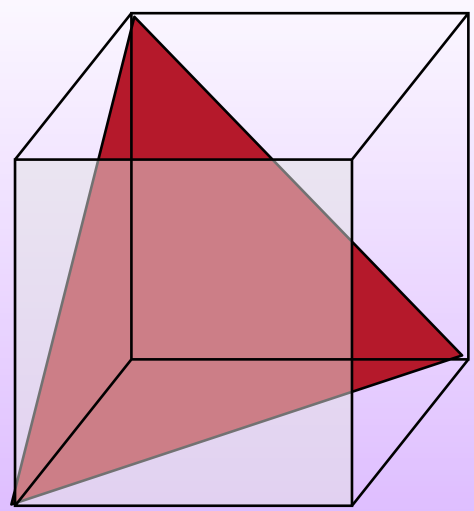
Intercepts → 1 ∞ ∞
Plane → (100)
Family → {100} → 6





Intercepts → 1 1 ∞
Plane → (110)
Family → {110} → 6

The purpose of using reciprocal of intercepts and not intercepts themselves in Miller indices becomes clear → the ∞ are removed



Intercepts → 1 1 1
Plane → (111)
Family → {111} → 8
(Octahedral plane)

Points about planes and directions

- Unknown/general direction → [uvw]
  - Corresponding family of directions → <uvw>
- Unknown/general plane → (hkl)
  - Corresponding family of planes → {hkl}
- Double digit indices should be separated by commas → (12,22,3) or (12 22 3)
- In cubic lattices/crystals [hkl] ⊥ (hkl). E.g. [111] ⊥ (111).

Interplanar spacing (d_{hkl}) in cubic lattice (& crystals)

$$d_{hkl}^{cubic\ lattice} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

Funda Checks

- **What does the 'symbol' (111) mean/represent?**

  The symbol (111) represents Miller indices for an *infinite set of parallel planes*, with intercepts 1, 1 & 1 along the three crystallographic axis (unit lattice parameter along these), *which pass through lattice points*.

- **(111) is the Miller indices for a plane (?)** *(to reiterate)*

  ➢ It is usually for an infinite set of parallel planes, with a specific 'd' spacing. Hence, (100) plane is no different from a (–100) plane (i.e. a set consists of planes related by translational symmetry).

  However, the outward normals for these two planes are different.

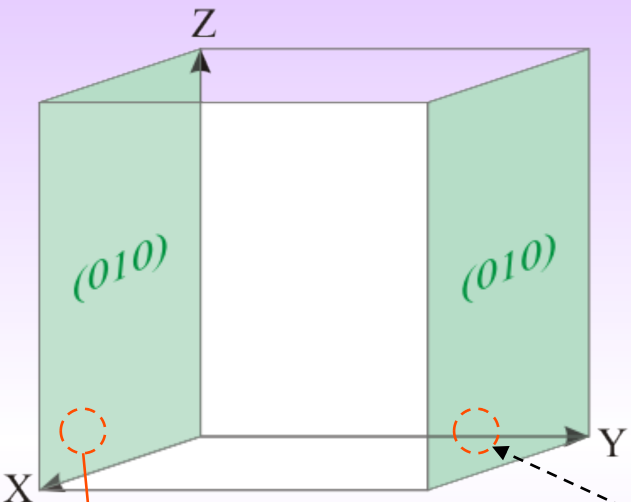
  Sometimes, it is also used for a specific plane.

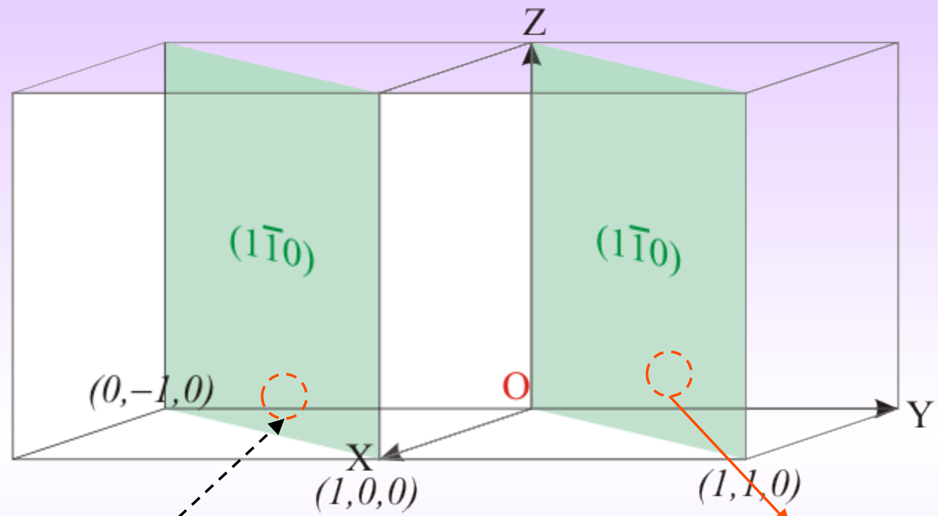
- **Are the members of the family of {100} planes: (100), (010), (001), (–100), (0–10), (00–1)?**

  ➢ This is a meaningless question without specifying the symmetry of the crystal. The above is true if one is referring to a crystal with (say) $\frac{4}{m}\bar{3}\frac{2}{m}$ symmetry. A 'family' is a symmetrically related set *(except for translational symmetry– which is anyhow part of the symbol (100))*.

Funda Check

- What about the plane passing through the origin?





Plane passing through origin

Plane passing through origin

Intercepts → ∞ 0 ∞
Plane → (0 ∞ 0)

Hence use this plane

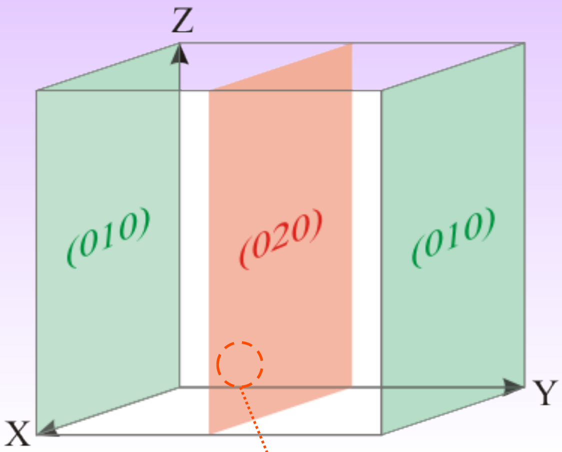
Intercepts → 0 0 ∞
Plane → (∞ ∞ 0)

We want to avoid infinities in Miller indices

In such cases the plane is translated by a unit distance along the non zero axis/axes and the Miller indices are computed

Funda Check

- What about planes passing through fractional lattice spacings?
  (We will deal with such fractional intersections with axes in X-ray diffraction).



$$d_{010}^{cubic\ lattice} = \frac{a}{\sqrt{0^2+1^2+0^2}} = a$$

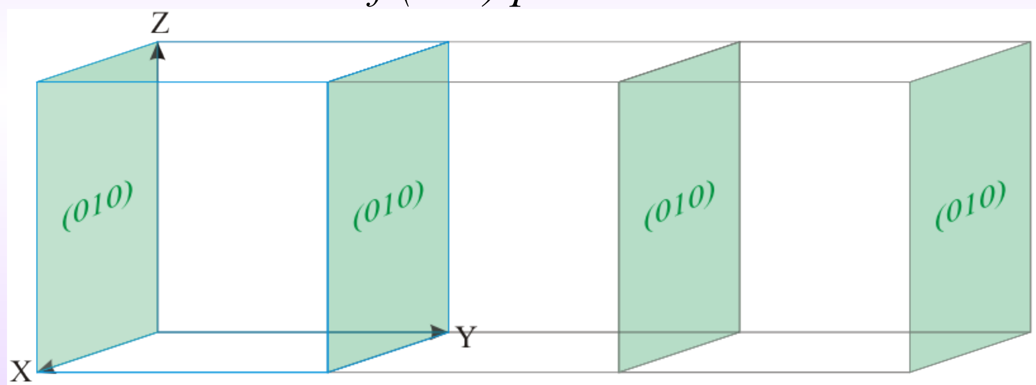
$$d_{020}^{cubic\ lattice} = \frac{a}{\sqrt{0^2+2^2+0^2}} = \frac{a}{2}$$

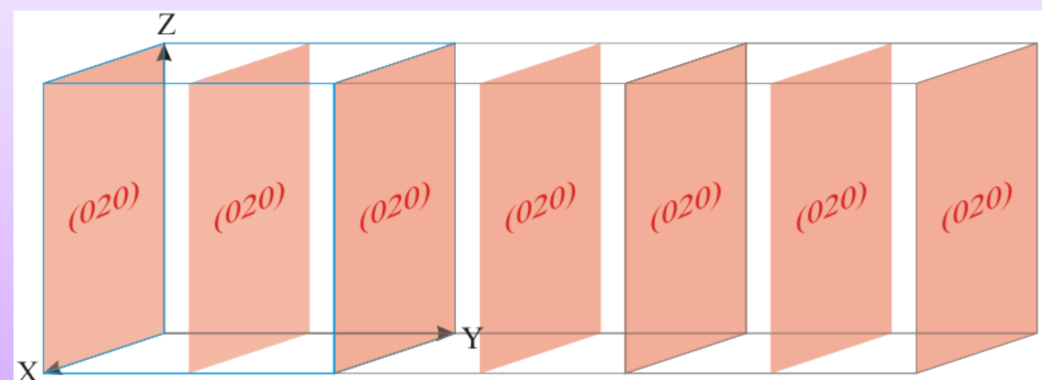
$$d_{020} = \frac{d_{010}}{2}$$

(020) has half the spacing as (010) planes

Intercepts → ∞ ½ ∞
Plane → (0 2 0)

Actually (020) is a superset of planes as compared to the set of (010) planes





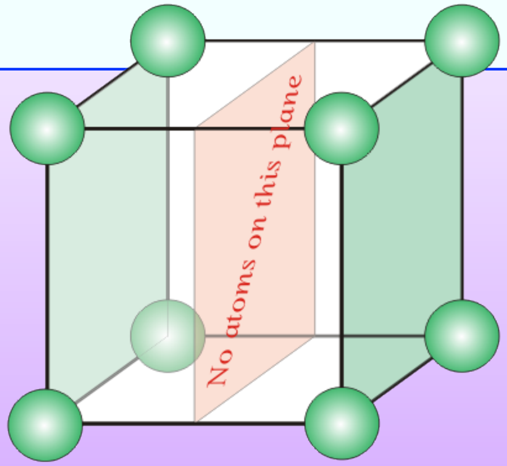
Note: in Simple cubic lattice this plane will not pass through lattice points!! But then lattice planes have to pass through lattice points!

Why do we consider such planes? We will stumble upon the answer later.

Funda Check

- Why talk about (020) planes? Isn't this the same as (010) planes as we factor out common factors in Miller indices?

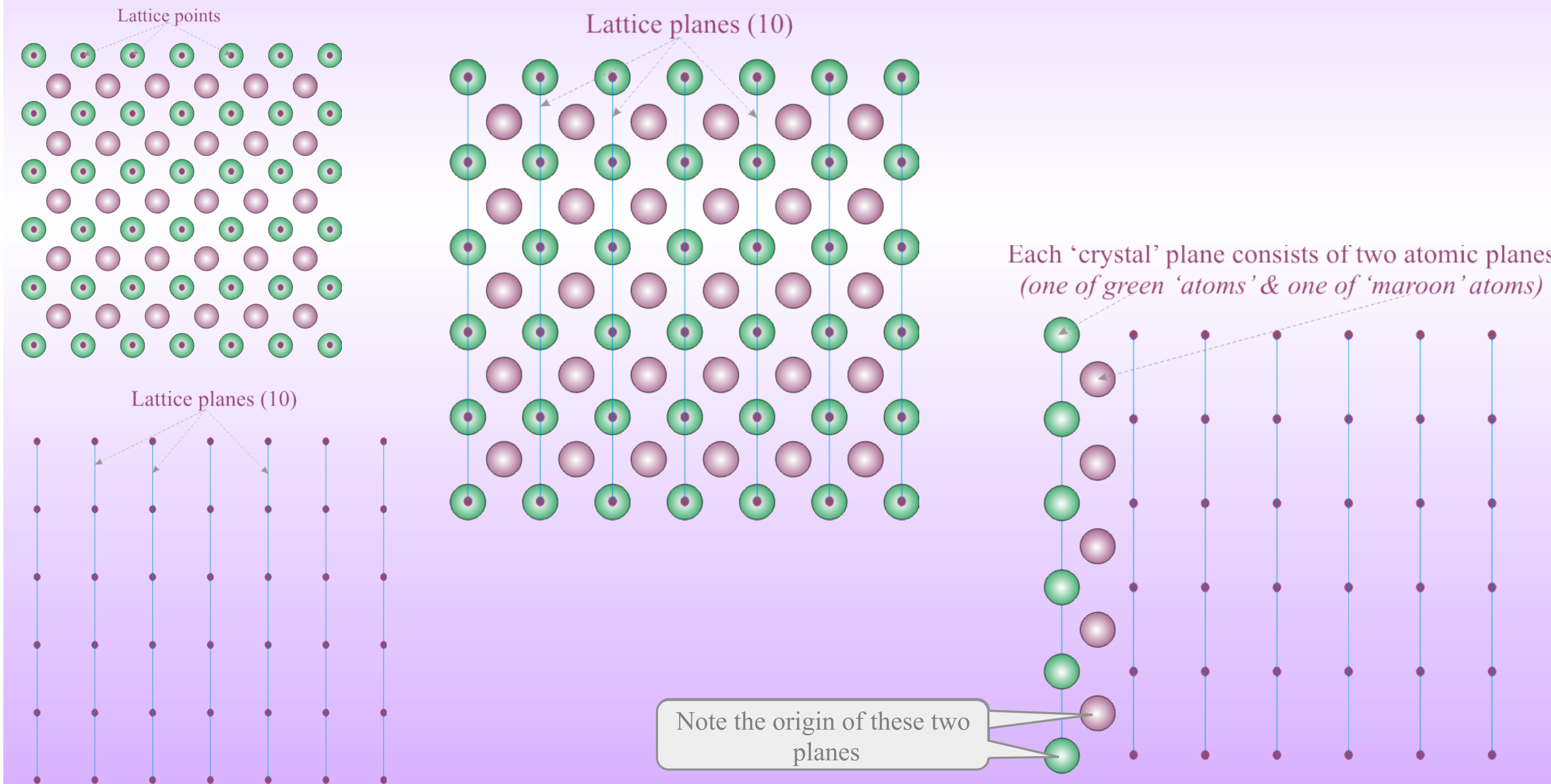
- Yes, in Miller indices we usually factor out the common factors.
- Suppose we consider a simple cubic crystal, *then alternate (020) planes will not have any atoms in them! (And this plane will not pass through lattice points as planes are usually required to do)*.
- Later, when we talk about x-ray diffraction then second order 'reflection' from (010) planes are often considered as first order reflection from (020) planes. This is (one of) the reason we need to consider (020) {or for that matter (222)≡2(111), (333), (220)} kind of planes.
- Similarly we will also talk about ½[110] kind of directions. The ½ in front is left out to emphasize the length of the vector (given by the direction). I.e. we are *not only* concerned about a direction, but also the length represented by the vector.



Funda Check

- In the crystal below what does the (10) plane contain? Using an 2D example of a crystal.

- The 'Crystal' plane (10) can be thought of consisting of 'Lattice' plane (10) + 'Motif' plane (10). I.e. the (10) crystal plane consists of two atomic planes associated with each lattice plane.
- This concept can be found not only in the superlattice example give below, but also in other crystals. E.g. in the CCP Cu crystal (110) crystal plane consists of two atomic planes of Cu.



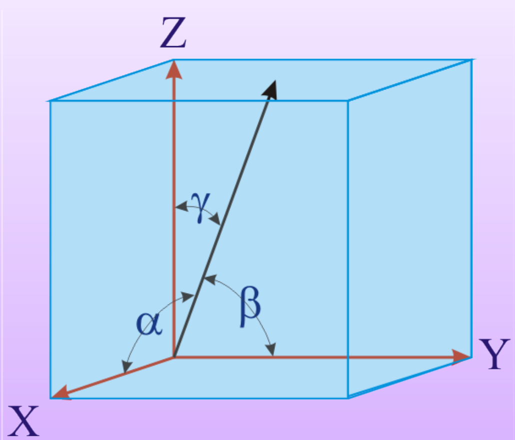
Funda Check

- Why do we need 3 indices (say for direction) in 3-dimensions?

- A direction in 3D can be specified by three angles- or the three direction cosines.
- There is one equation connecting the three direction cosines:

$$Cos^2\alpha + Cos^2\beta + Cos^2\gamma = 1$$

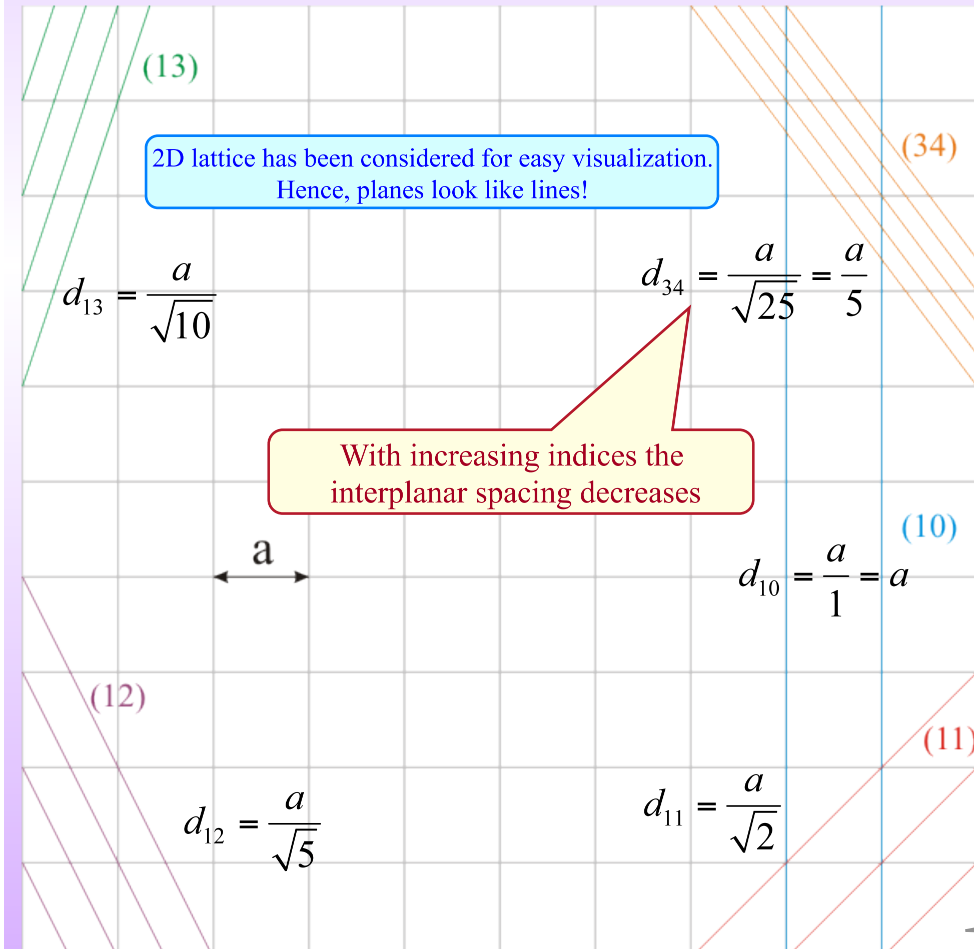
- This implies that we required only two independent parameters to describe a direction. *Then why do we need three Miller indices?*
- The Miller indices prescribe the direction as a vector having a particular length (i.e. this prescription of length requires the additional index)
- Similarly three Miller indices are used for a plane (hkl) as this has additional information regarding interplanar spacing. E.g.: $d_{hkl}^{cubic\ lattice} = \dfrac{a}{\sqrt{h^2 + k^2 + l^2}}$



Funda Check

1) What happens to d_{hkl} with increasing hkl?
2) Can planes have spacing less than inter-atomic spacings?
3) What happens to lattice density (no. of lattice points per unit area of plane)?
4) What is meant by the phrase: 'planes are imaginary'?

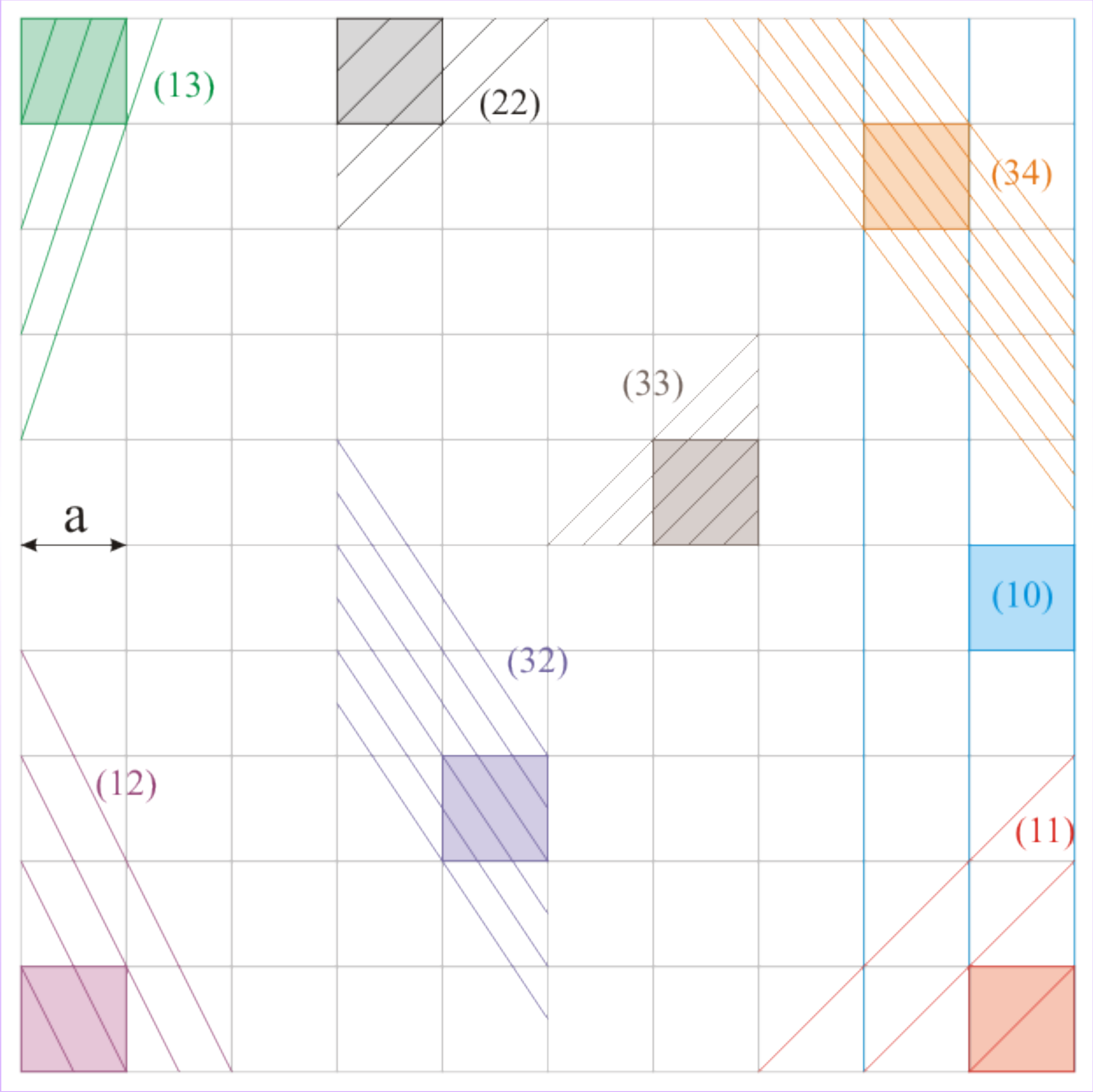
1) As *h,k,l* increases, 'd' decreases ⇒ we could have planes with *infinitesimal* spacing.
2) The above implies that inter-planar spacing could be much less than inter-atomic spacing.



3) With increasing indices (h,k,l) the lattice density (or even motif density) decreases. (in 2D lattice density is measured as no. of lattice points per unit length).
   - E.g. the (10) plane has 1 lattice point for length 'a', while the (11) plane has 1 lattice point for length a√2 *(i.e. lower density)*.
4) Since we can *draw any number of planes* through the same lattice (as in the figure), clearly the concept of a lattice plane (or for that matter a crystal plane or a lattice direction) is a 'mental' construct (imaginary).

Note: the grey lines do not mean anything (consider this to be a square lattice)

1 more view with more planes and unit cell overlaid



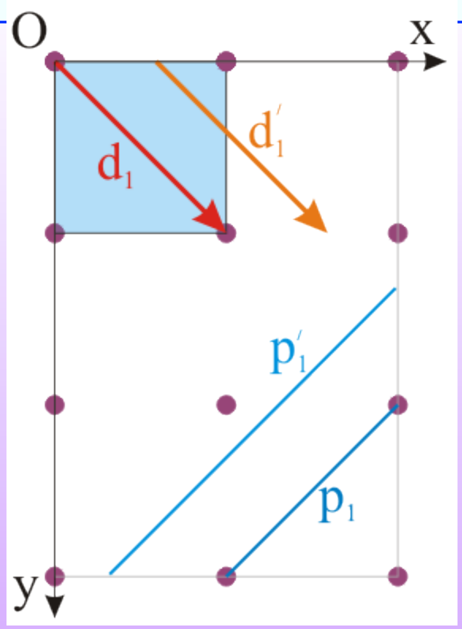
In an upcoming slide we will see how a (hkl) plane will divide the edge, face diagonal and body diagonal of the unit cell

In this 2D version you can already note that diagonal is divided into (h + k) parts

Funda Check

- Do planes and directions have to pass through lattice points?

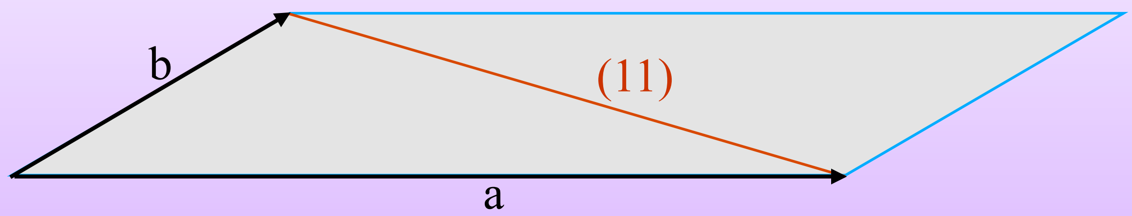
- In the figure below a direction and plane are marked.
- In principle d_1 and d_1' are identical vectorally- but they are positioned differently w.r.t to the origin.
- Similarly planes p_1 and p_1' are identical except that they are positioned differently w.r.t to the coordinate axes.
- In crystallography we usually use d_1 and p_1 *(those which pass through lattice points)* and do not allow any parallel translations (which leads to a situation where these do not pass through lattice points) .
- We have noted earlier that Miller indices (say for planes) contains information about the interplanar spacing and hence the convention.



Funda Check

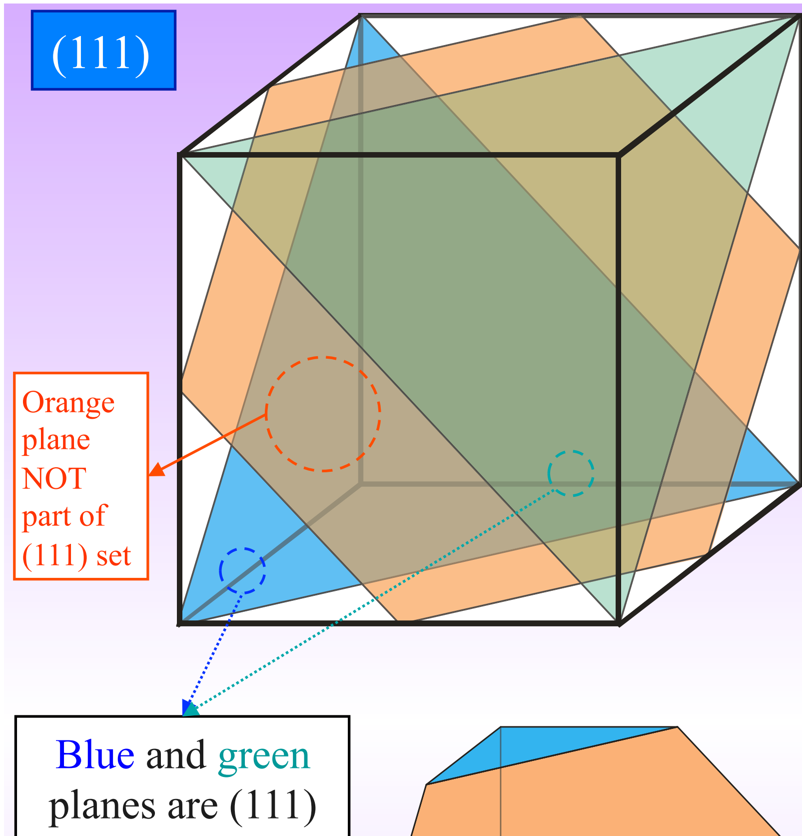
- For a plane (11) what are the *units* of the intercepts?

- Here we illustrate the concept involved using the (11) plane, but can be applied equally well to directions as well.
- The (11) plane has intercepts along the crystallographic axis at (1,0) and (0,1).
- In a given lattice/crystal the ‘a’ and ‘b’ axis need not be of equal length (further they may be inclined to each other). This implies that thought the intercepts are one unit along ‘a’ and ‘b’, their physical lengths may be very different (as in the figure below).



(111)

Further points about (111) planes

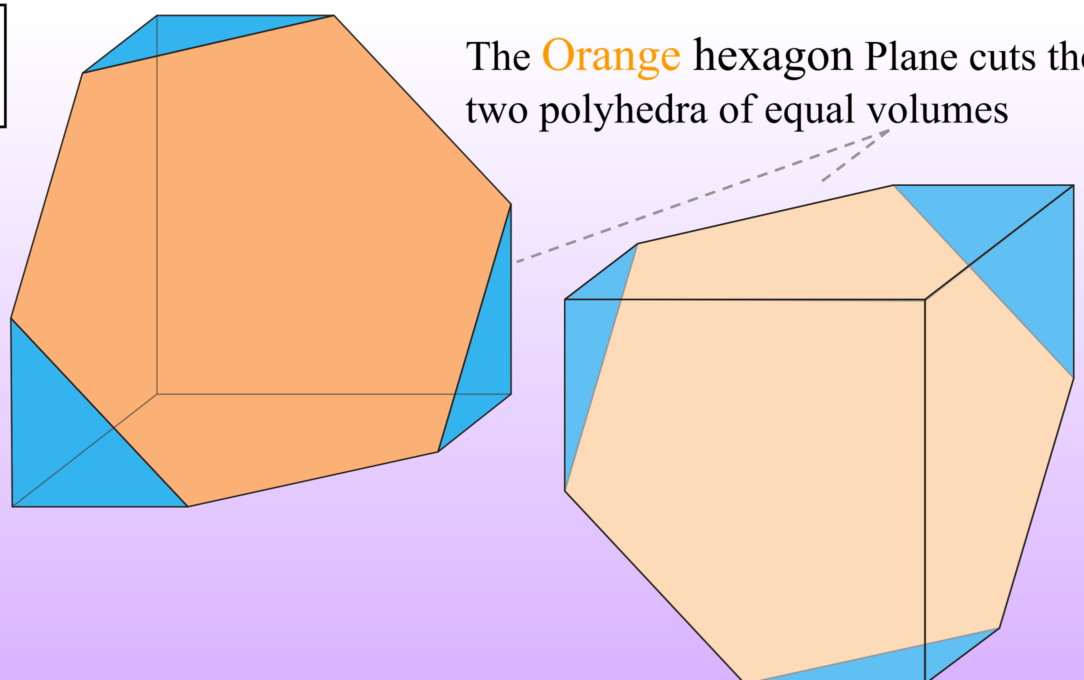


Family of {111} planes within the cubic unit cell (Light green triangle and light blue triangle are (111) planes within the unit cell).
The Orange hexagon is parallel to these planes.

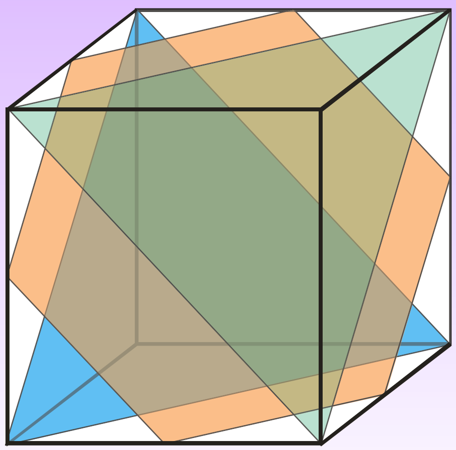
$$d_{(111)} = a/\sqrt{3} = a\sqrt{3}/3 = \frac{Body\ diagonal\ length}{3}$$

The (111) plane trisects the body diagonal

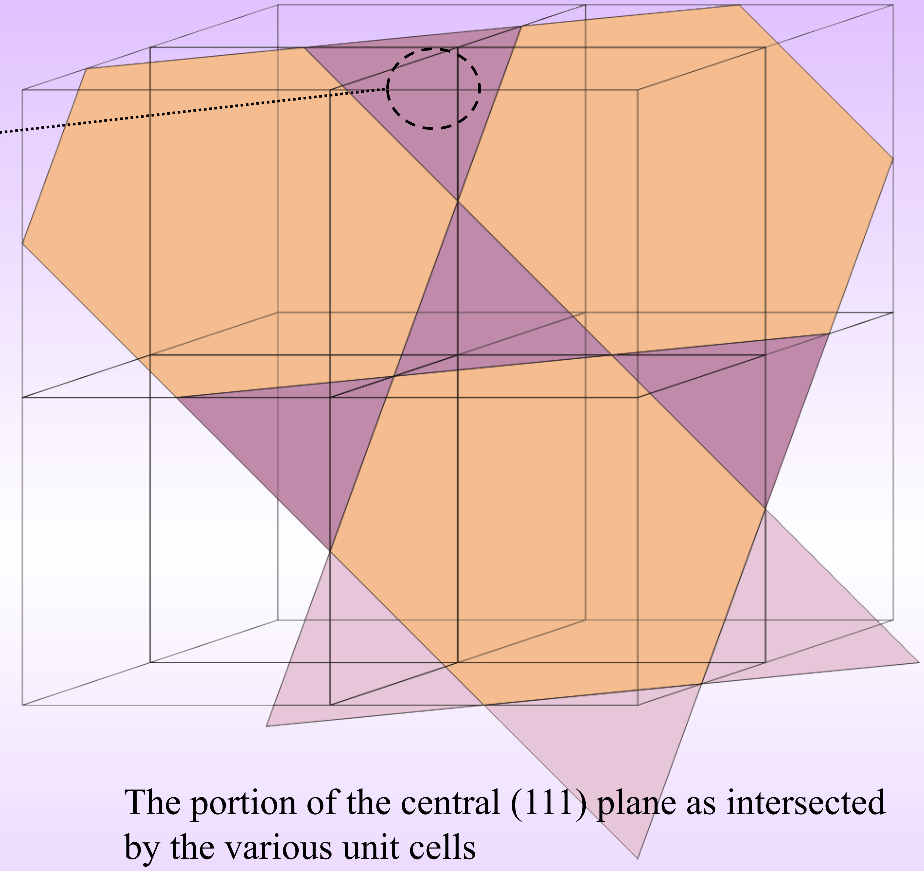
The Orange hexagon Plane cuts the cube into two polyhedra of equal volumes



The central (111) plane (orange colour) is not a 'space filling' plane!



Portion of the (111) plane not included within the unit cell

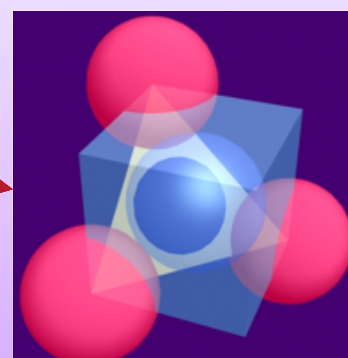


The portion of the central (111) plane as intersected by the various unit cells

Suppose we want to make a calculation of areal density (area fraction occupied by atoms) of atoms on the (111) plane- e.g. for a BCC crystal.

Q) Can any of these (111) planes be used for the calculation?

A) If the calculation is being done within the unit cell then the central orange plane cannot be used as it (the hexagonal portion) is *not* space filling → as shown in the figure on the right.



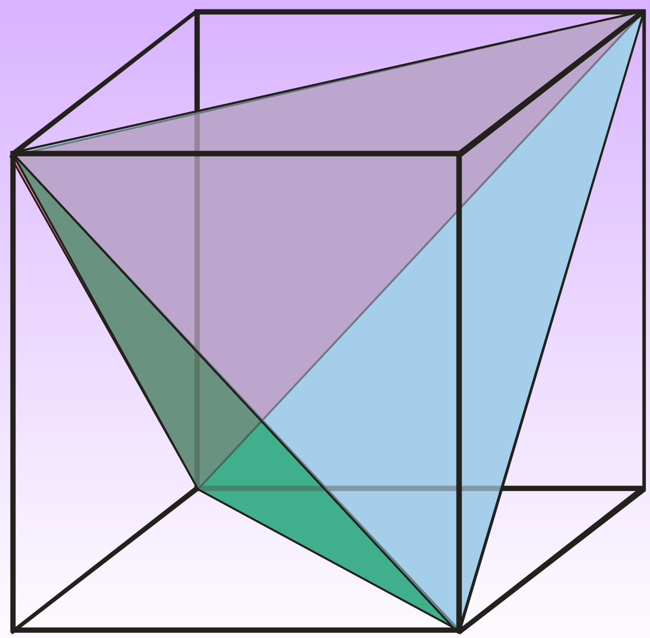
Video: (111) plane in BCC crystal

Low resolution

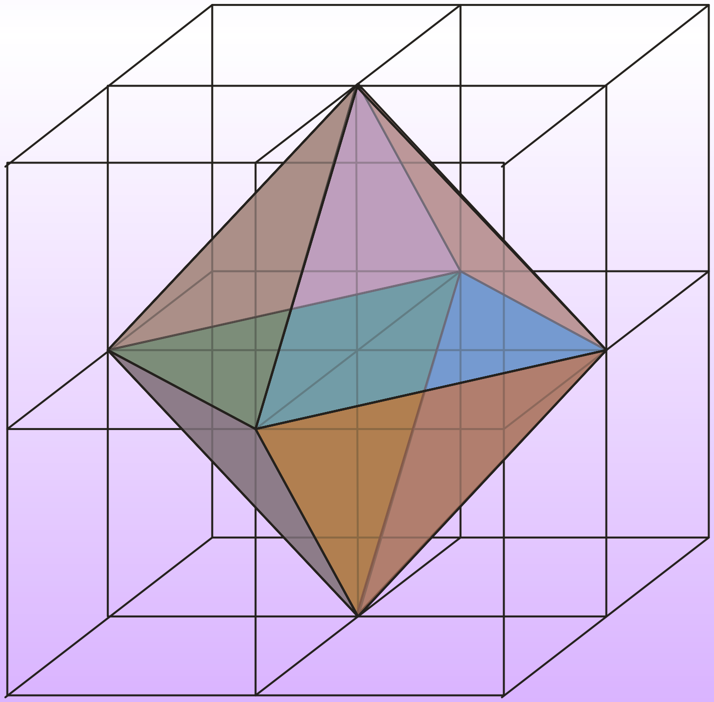
Video: (111) plane in BCC crystal

Solved Example

What is the true areal fraction of atoms lying in the (111) plane of a BCC crystal?



Tetrahedron inscribed inside a cube with bounding planes belonging to the $\{111\}_{\text{cubic lattice}}$ family (subset of the full family)



8 planes of $\{111\}_{\text{cubic lattice}}$ family forming a regular octahedron

Members of a family of planes in cubic crystal/lattice

Index	Number of members in a cubic lattice	d_{hkl}	
{100}	6	$d_{100} = a$	
{110}	12	$d_{110} = a/\sqrt{2} = a\sqrt{2}/2$	The (110) plane bisects the face diagonal
{111}	8	$d_{111} = a/\sqrt{3} = a\sqrt{3}/3$	The (111) plane trisects the body diagonal
{210}	24		
{211}	24		
{221}	24		
{310}	24		
{311}	24		
{320}	24		
{321}	48		

Summary of notations

	Symbol		Alternate symbols		
Direction	[ ]	[uvw]		→	Particular direction
	< >	<uvw>	[[ ]]	→	Family of directions
Plane	( )	(hkl)		→	Particular plane
	{ }	{hkl}	(( ))	→	Family of planes
Point	. .	.xyz.	[[ ]]	→	Particular point
	: :	:xyz:		→	Family of point

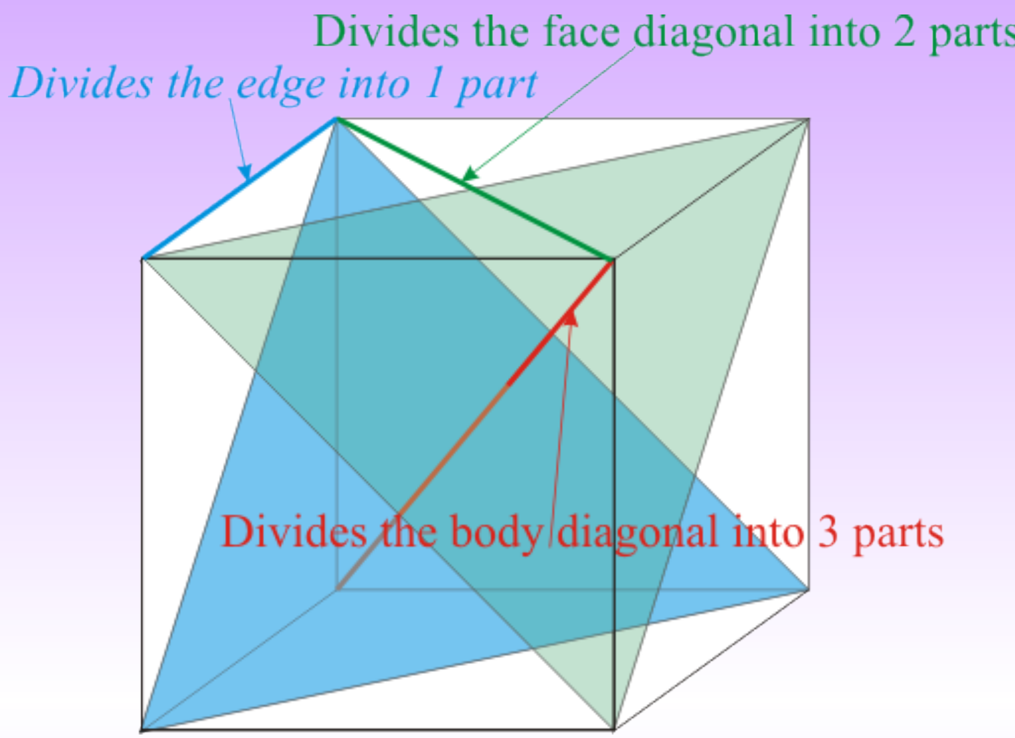
A family is also referred to as a symmetrical set

Points about (hkl) planes

For a set of translationally equivalent lattice planes will divide:

Entity being divided *(Dimension containing the entity)*		Direction	number of parts
Cell edge *(1D)*	a	[100]	h
	b	[010]	k
	c	[001]	l
Diagonal of cell face *(2D)*	(100)	[011]	(k + l)
	(010)	[101]	(l + h)
	(001)	[110]	(h + k)
Body diagonal *(3D)*		[111]	(h + k + l)

The (111) planes:



In general

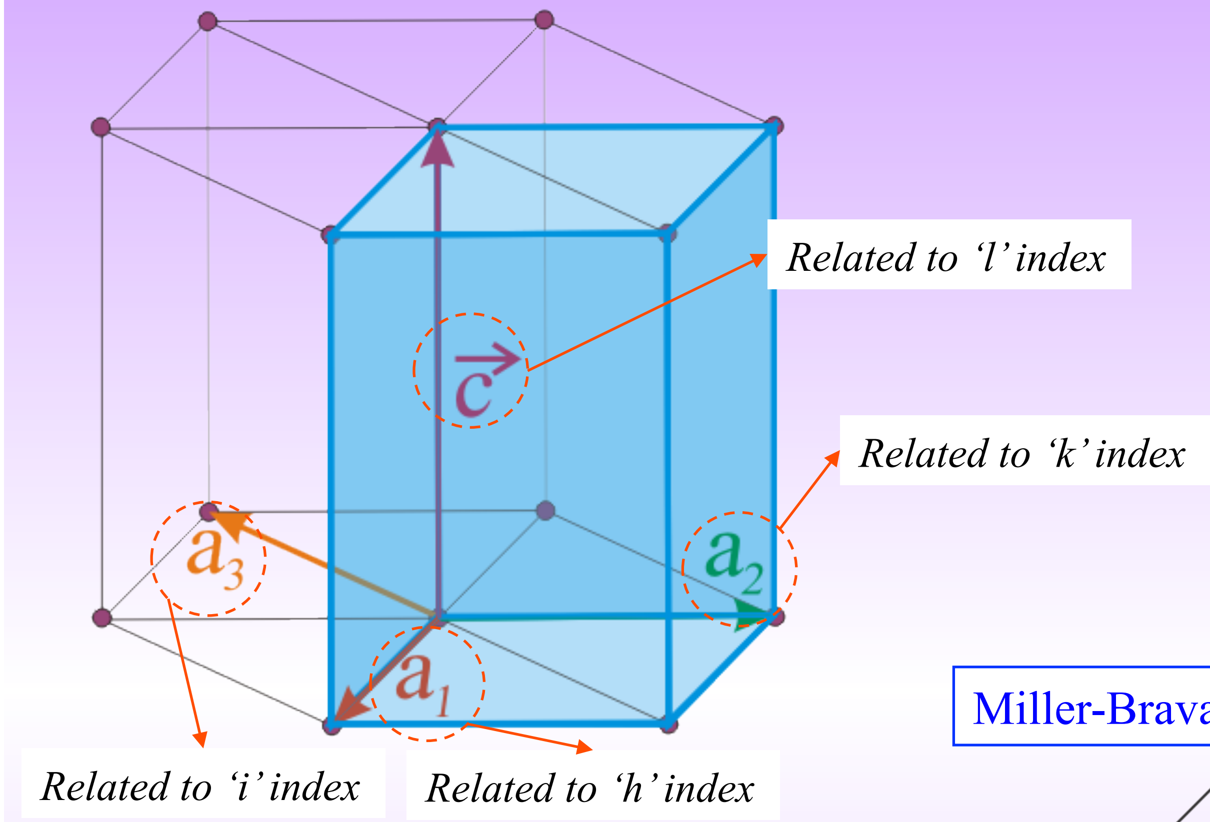
Condition	(hkl) will pass through
h even	midpoint of a
(k + l) even	face centre (001) midpoint of face diagonal (001)
(h + k + l) even	body centre midpoint of body diagonal

Hexagonal crystals → Miller-Bravais Indices

- Directions and planes in hexagonal lattices and crystals are designated by the 4-index Miller-Bravais notation.
- The Miller-Bravais notation can be a little tricky to learn.
- 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* (which can be derived from the first two as in the formula below) and is introduced to make sure that members of a family of directions or planes have a set of numbers which are identical
  - this is because in 2D two indices *suffice* to describe a lattice (or crystal)
  - the fourth index represents the 'c' axis *(⊥ to the basal plane)*.
- Hence the first three indices in a hexagonal lattice can be permuted to get the different members of a family; while, the fourth index is kept separate.

(h k i l)

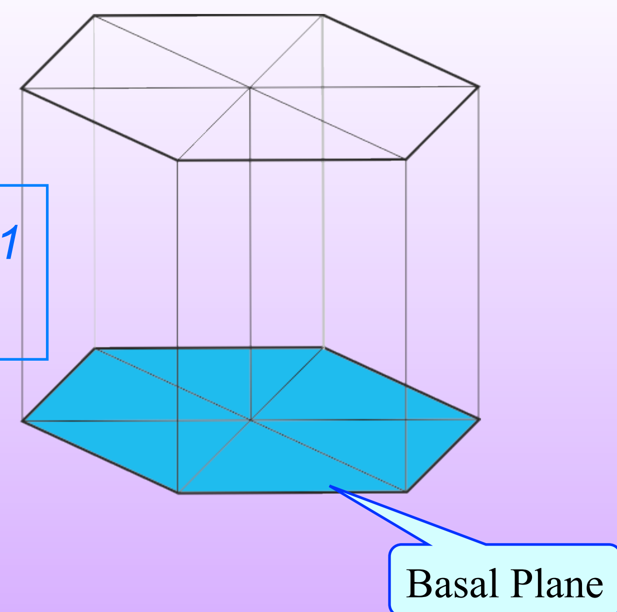
$$\mathbf{i = -(h + k)}$$



Miller-Bravais Indices for the Basal Plane

Intercepts → ∞ ∞ ∞ 1

Plane → (0 0 0 1)

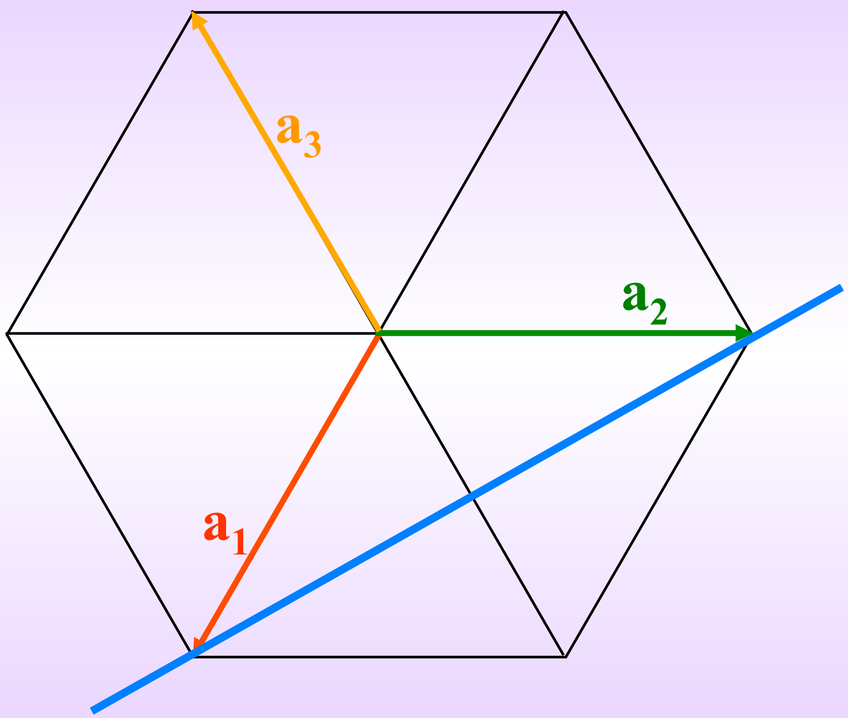


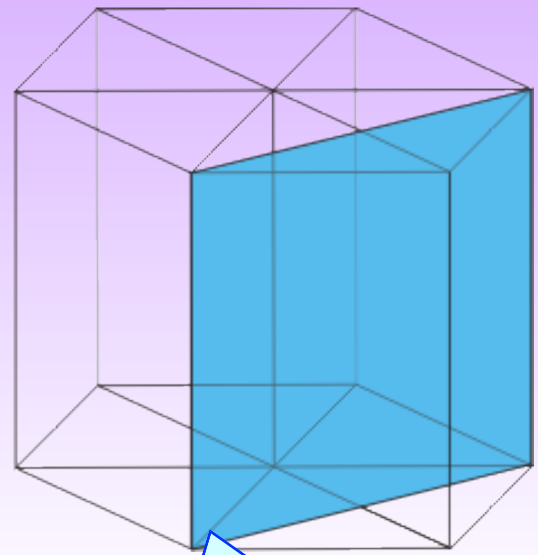
Intercepts → 1 1 - ½ ∞

Plane → (1 1 $\bar{2}$ 0)

(h k i l)

i = -(h + k)

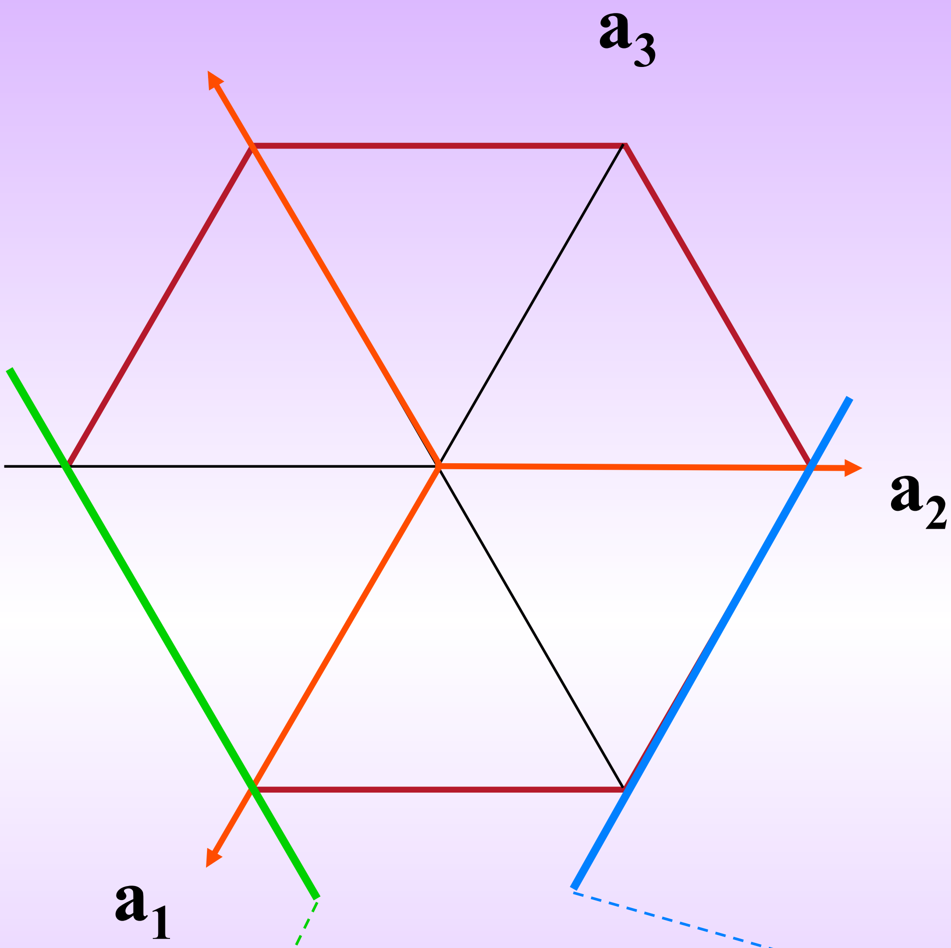




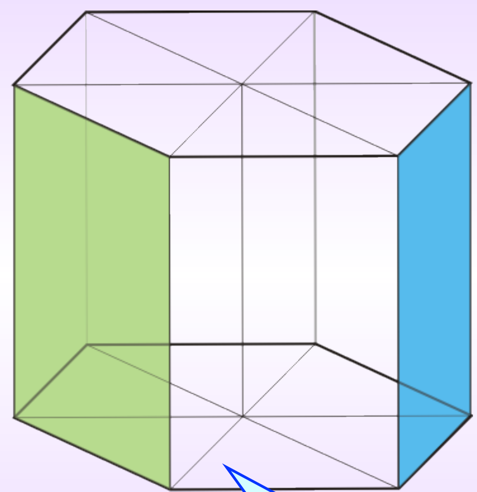
Planes which have ∞ intercept along c -axis (i.e. vertical planes) are called Prism planes

The use of the 4 index notation is to bring out the equivalence between crystallographically equivalent planes and directions (as will become clear in coming slides)

Examples to show the utility of the 4 index notation



Obviously the 'green' and 'blue' planes belong to the same family and first three indices have the same set of numbers (as brought out by the Miller-Bravais system)

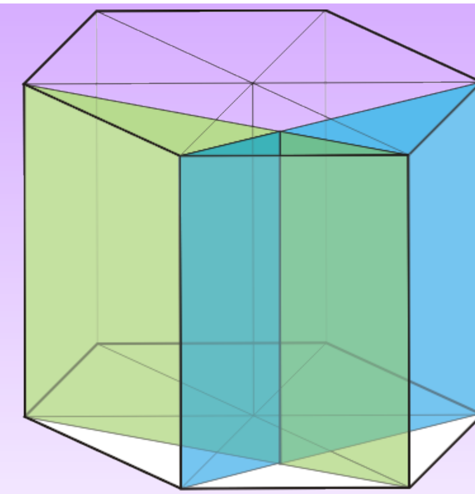


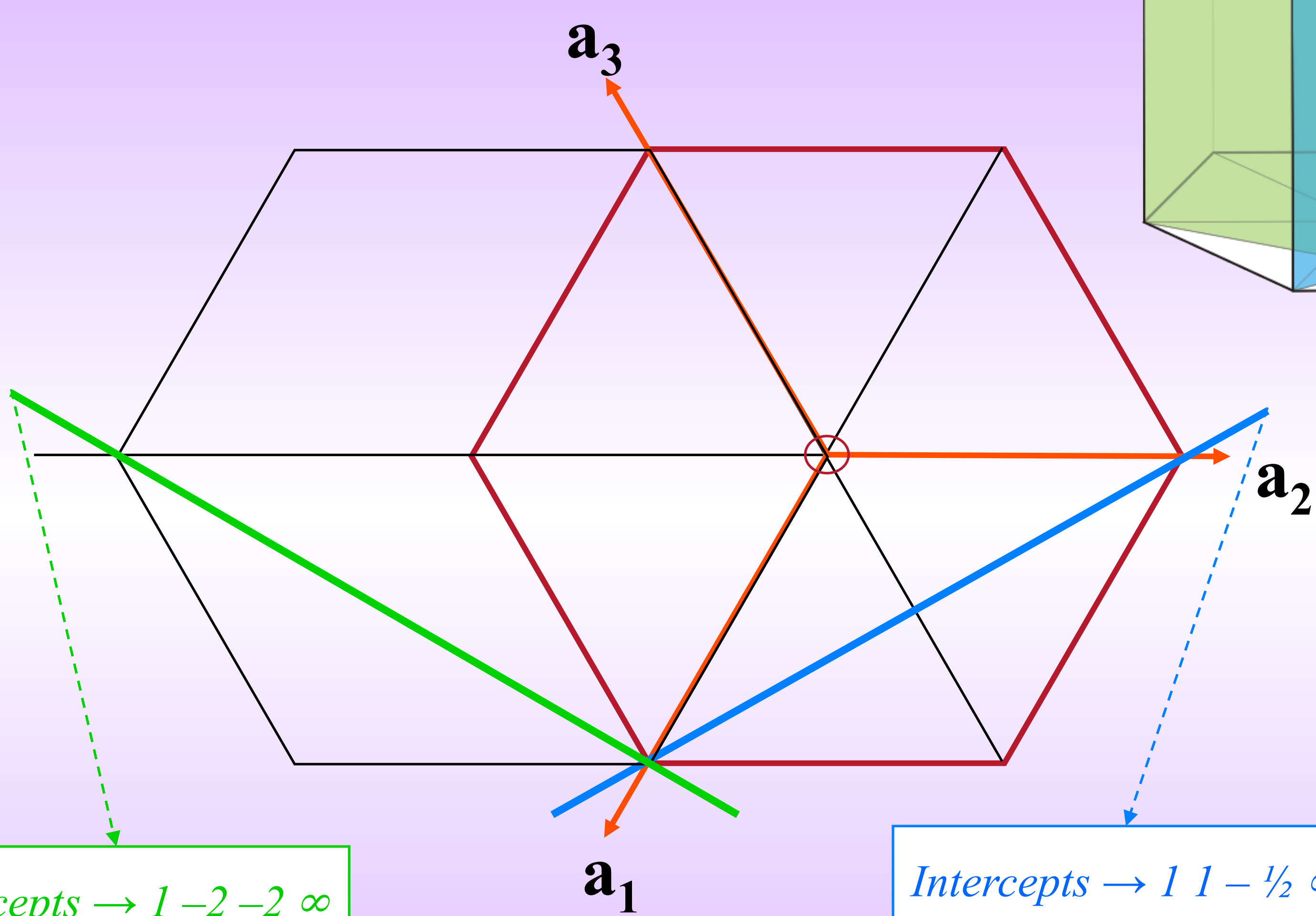
Planes which have ∞ intercept along c-axis (i.e. vertical planes) are called Prism planes

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)

Examples to show the utility of the 4 index notation



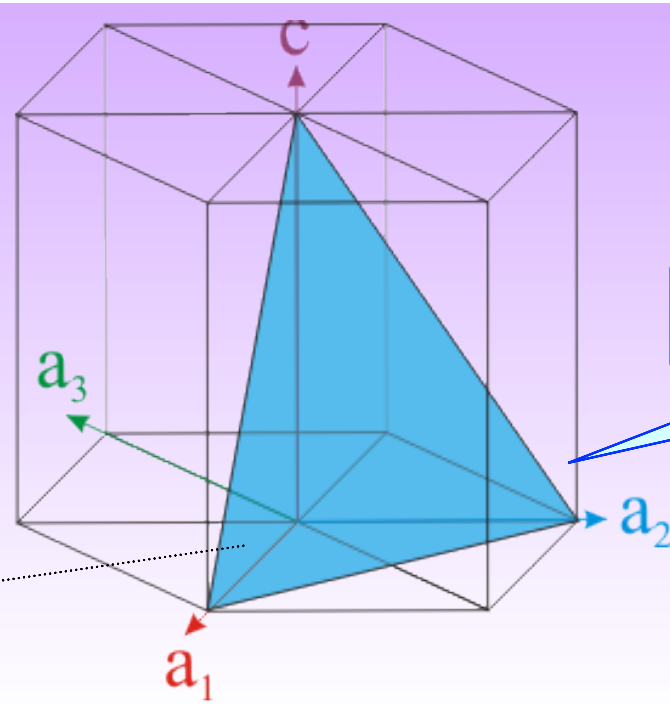


Intercepts → 1 –2 –2 ∞

Plane → (2 ▯1 ▯1 0)

Intercepts → 1 1 – ½ ∞

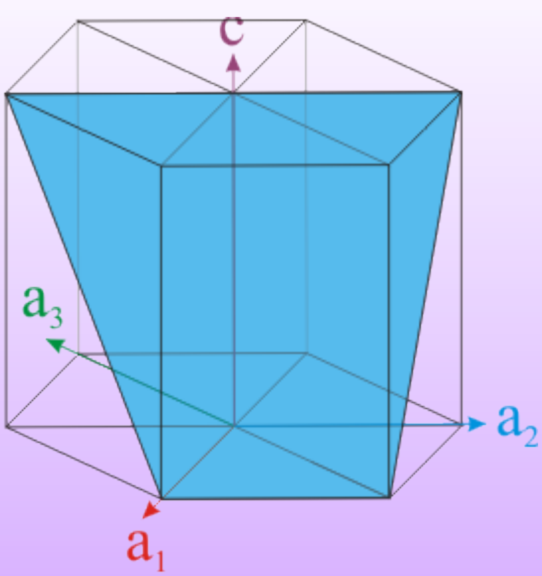
Plane → (1 1 ▯2 0)

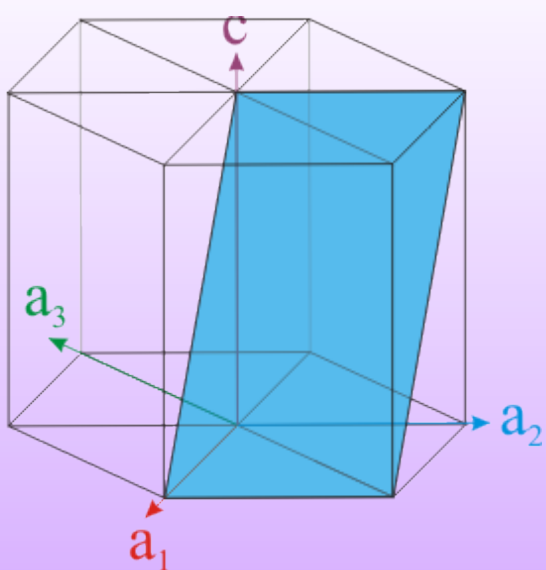


Inclined planes which have finite intercept along c-axis are called Pyramidal planes

Intercepts → 1 1 - ½ 1

Plane → (1 1 $\bar{2}$ 1)



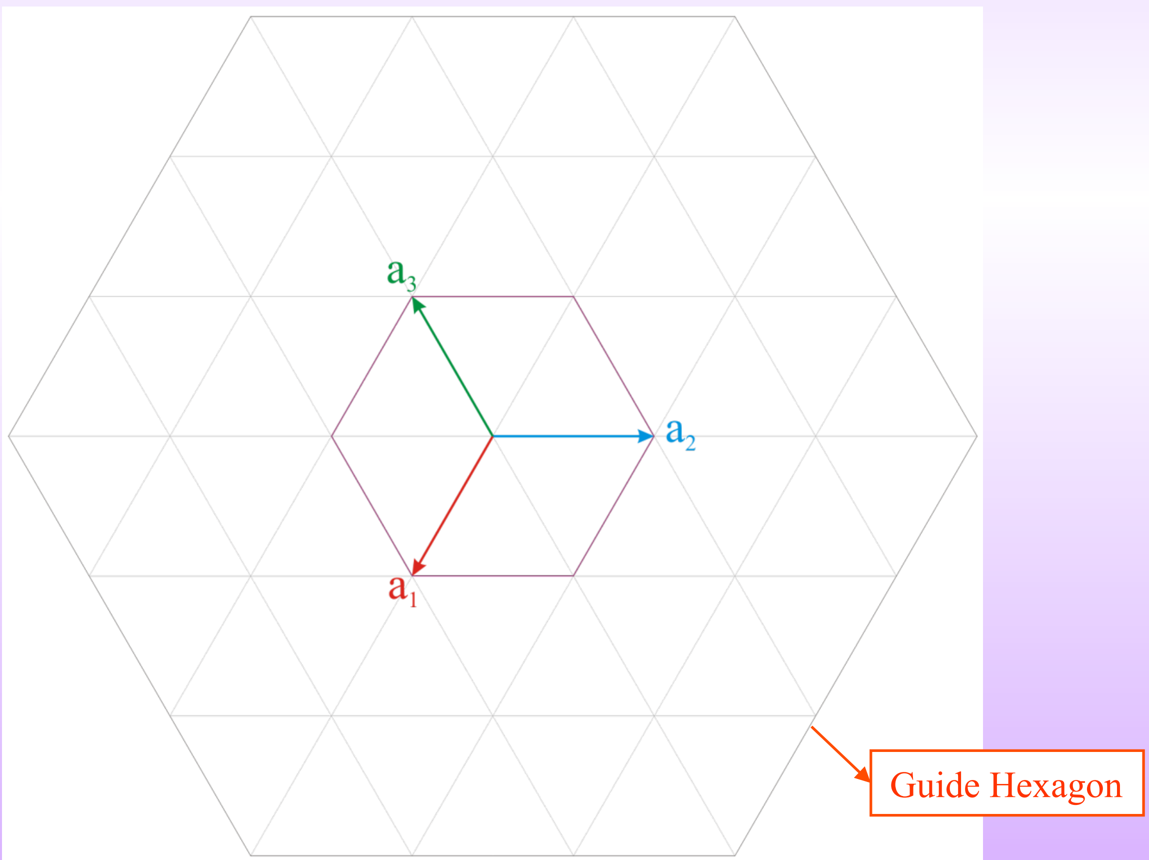


Intercepts → 1 ∞ - 1 1

Plane → (1 0 $\bar{1}$ 1)

Directions

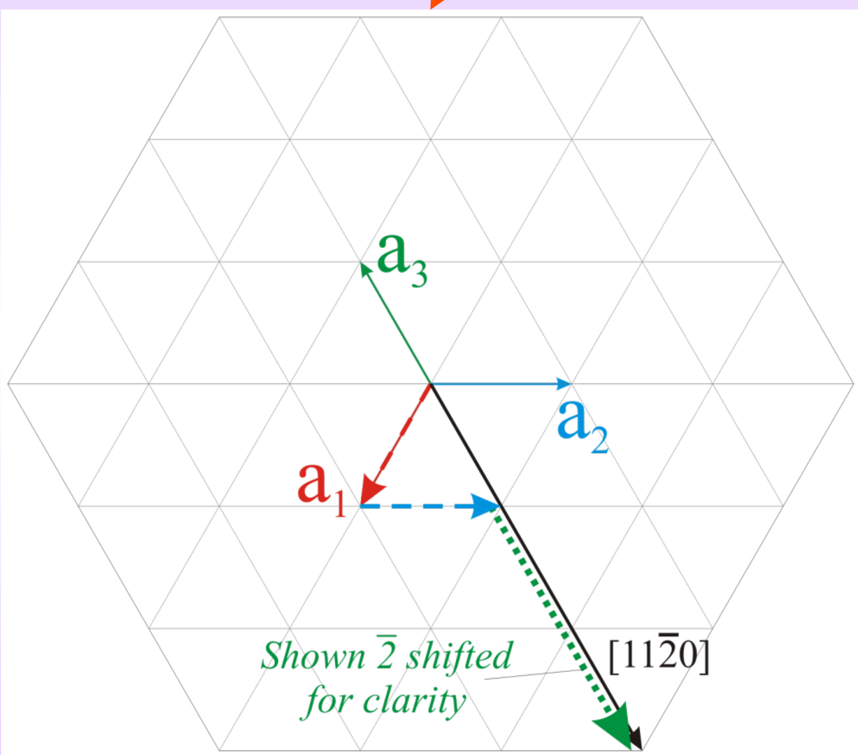
- One has to be careful in determining directions in the Miller-Bravais system.
- Basis vectors a_1, a_2 & a_3 are symmetrically related by a six fold axis.
- The 3[rd] index is redundant and is included to bring out the equality between equivalent directions (like in the case of planes).
- In the drawing of the directions we use an additional guide hexagon 3 times the unit basis vectors (a_i).



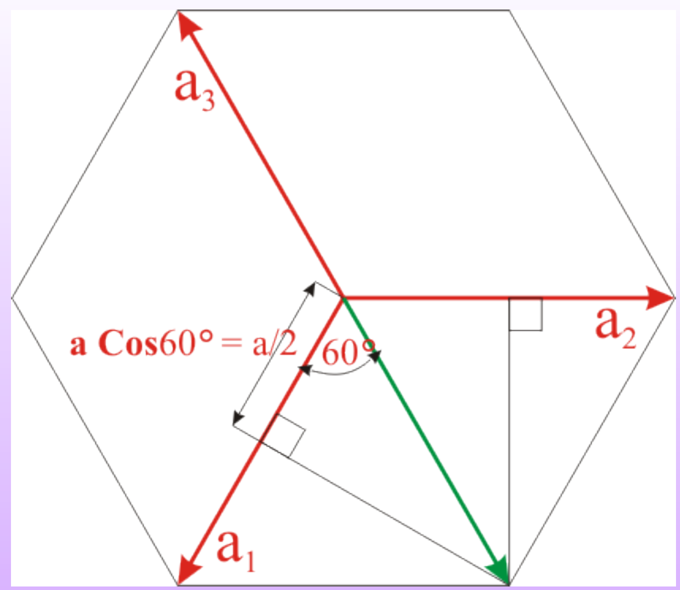
Directions

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

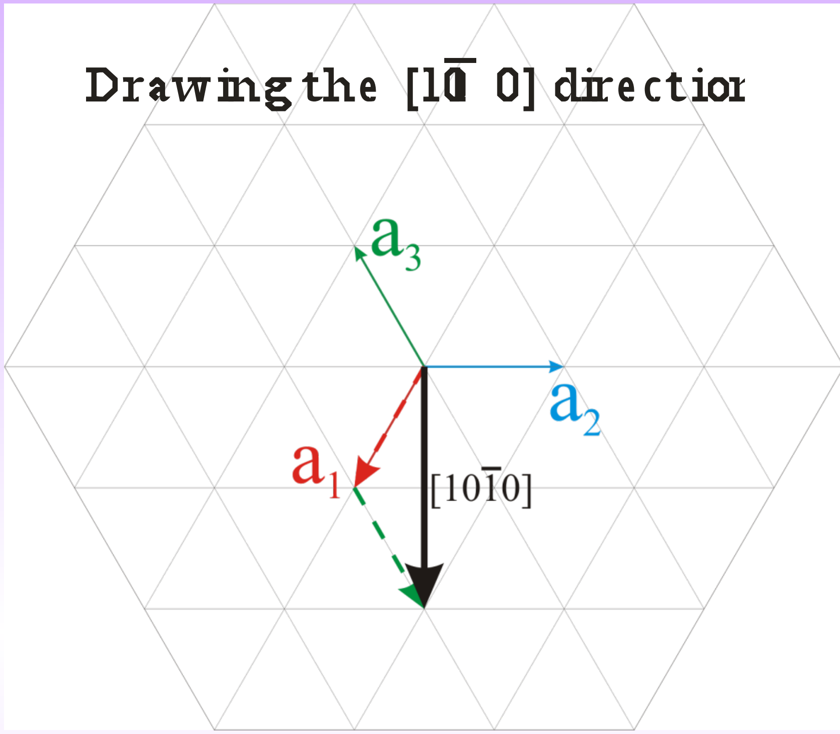
- Trace a path along the basis vectors as required by the direction. In the current example move 1unit along a_1, 1unit along a_2 and -2 units along a_3.
- Directions are projected onto the basis vectors to determine the components and hence the Miller-Bravais indices can be determined as in the table.



	a_1	a_2	a_3
Projections	a/2	a/2	−a
Normalized wrt LP	1/2	1/2	−1
Factorization	1	1	−2
Indices	[1 1 $\bar{2}$ 0]		

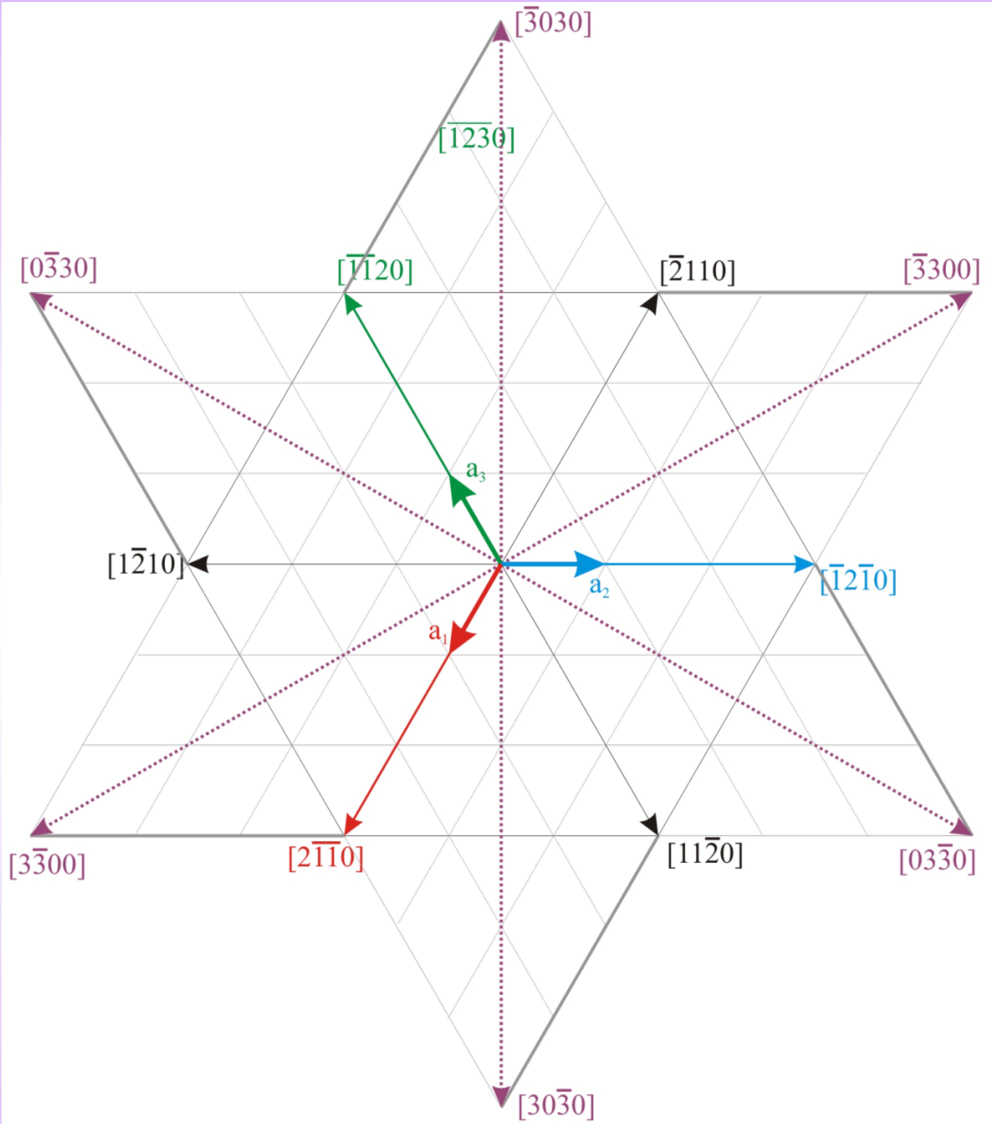


We do similar exercises to draw other directions as well



	a_1	a_2	a_3
Projections	3a/2	0	–3a/2
Normalized wrt LP	3/2	0	– 3/2
Factorization	1	0	−1
Indices	[1 0 –1 0]		

Some important directions



Overlaying planes and directions

- Note that for planes of the type (000l) or (hki0) are perpendicular to the respective directions [0001] or [hki0] → (000l) ⊥ [0001], (hki0) ⊥ [hki0].
- However, in general (hkil) is not perpendicular to [hkil], except if c/a ratio is $\sqrt{(3/2)}$.
- The direction perpendicular to a particular plane will depend on the c/a ratio and may have high indices or even be irrational.

Transformation between 3-index *[UVW]* and 4-index *[uvtw]* notations

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

$$u = \frac{1}{3}(2U - V) \qquad v = \frac{1}{3}(2V - U) \qquad t = -(u + v) \qquad w = W$$

- Directions in the hexagonal system can be expressed in many ways
- 3-indices:
  By the three vector components along a_1, a_2 and c:
  $r_{UVW} = Ua_1 + Va_2 + Wc$
- In the three index notation equivalent directions may not seem equivalent; while, in the four index notation the equivalence is brought out.

Weiss Zone Law

- If the Miller plane (hkl) contains *(or is parallel to)* the direction [uvw] then:

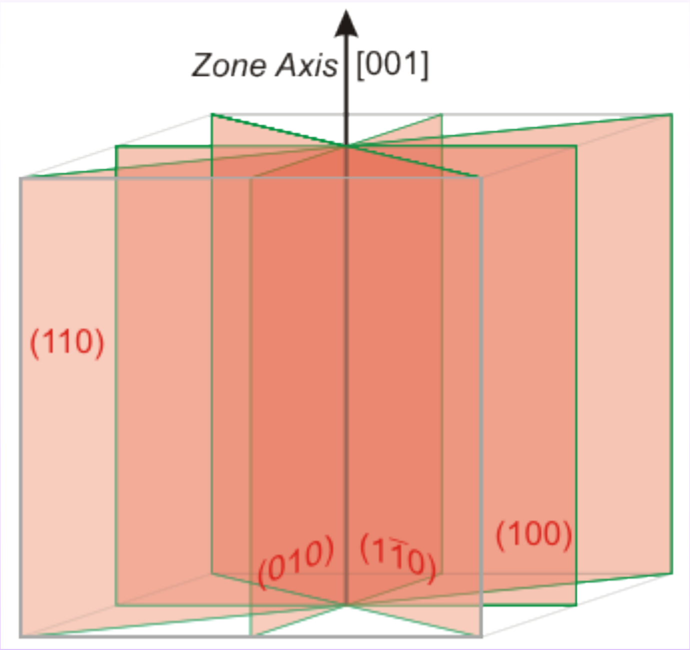
$$h.u + k.v + l.w = 0$$

- This relation is valid for all crystal systems *(referring to the standard unit cell).*

Solved Example

Zone Axis

- The direction common to a set of planes is called the zone axis of those planes.
- E.g. [001] lies on (110), (1-10), (100), (210) etc.
- If $(h_1\ k_1\ l_1)$ & $(h_2\ k_2\ l_2)$ are two planes having a common direction [uvw] then according to Weiss zone law:
  $u.h_1 + v.k_1 + w.l_1 = 0$ & $u.h_2 + v.k_2 + w.l_2 = 0$
- This concept is very useful in Selected Area Diffraction Patterns (SADP) in a TEM.



Note: Planes of a zone lie on a great circle in the stereographic projection

Directions ⊥ Planes

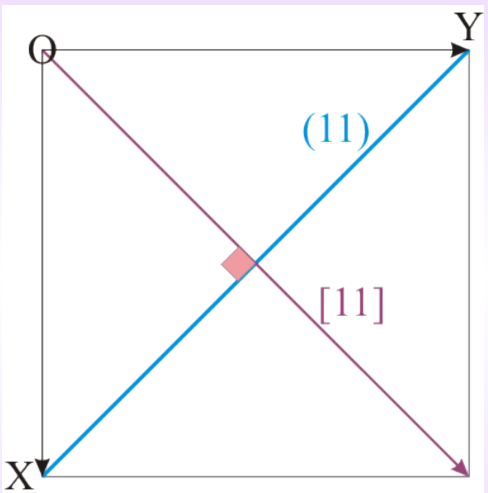
- Cubic system*: (hkl) ⊥ [hkl]
- Tetragonal system*: only special planes are ⊥ to the direction with same indices:
  [100] ⊥ (100), [010] ⊥ (010), [001] ⊥ (001), [110] ⊥ (110)
  ([101] not ⊥ (101))
- Orthorhombic system*:
  [100] ⊥ (100), [010] ⊥ (010), [001] ⊥ (001)
- Hexagonal system*: [0001] ⊥ (0001)
  ► *This is for a general c/a ratio*
  ► *For a Hexagonal crystal with the special c/a ratio = √(3/2)*
  → the cubic rule is followed (i.e. all planes are ⊥ to all directions)
- Monoclinic system*: [010] ⊥ (010)
- Other than these a general [hkl] is NOT ⊥ (hkl)

** Here we are referring to the conventional unit cell chosen (e.g. a=b=c, α=β=γ=90° for cubic) and not the symmetry of the crystal.*

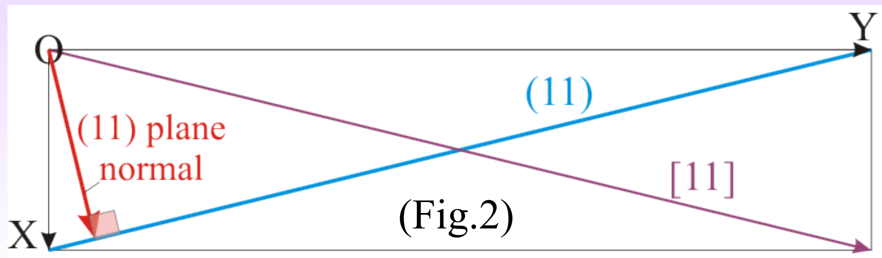
Funda Check

Which direction is perpendicular to which plane?

- In the cubic system all directions are perpendicular to the corresponding planes ((hkl) ⊥ [hkl]). 2D example of the same is given in the figure on the left (Fig.1).
- However, this is not universally true. To visualize this refer to Fig.2 and Fig.3 below.

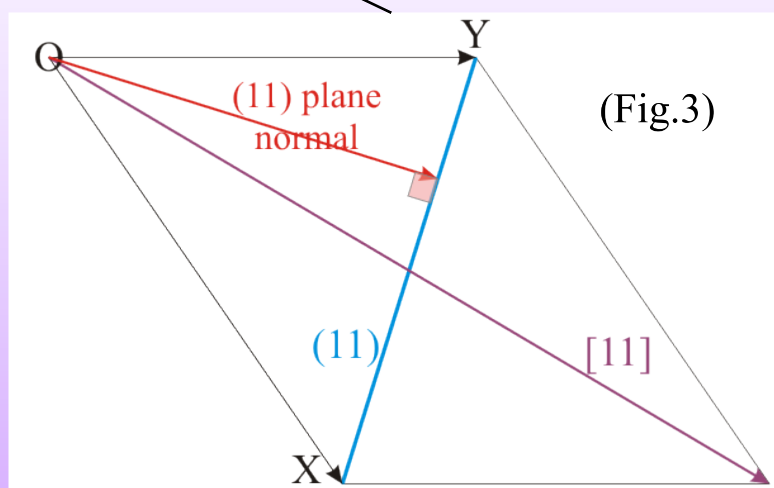


(Fig.1)



(Fig.2)

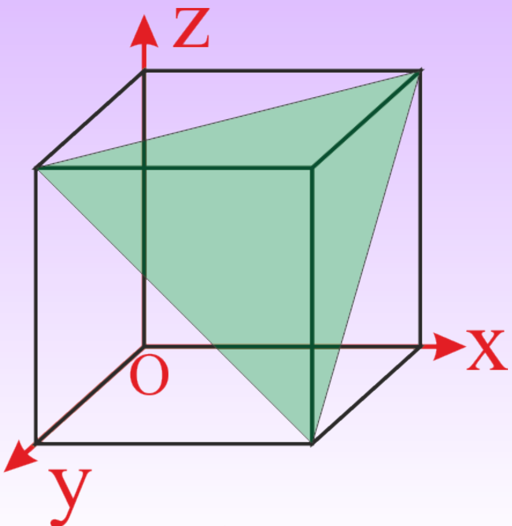
Note that plane normal to (11) plane is not the same as the [11] direction

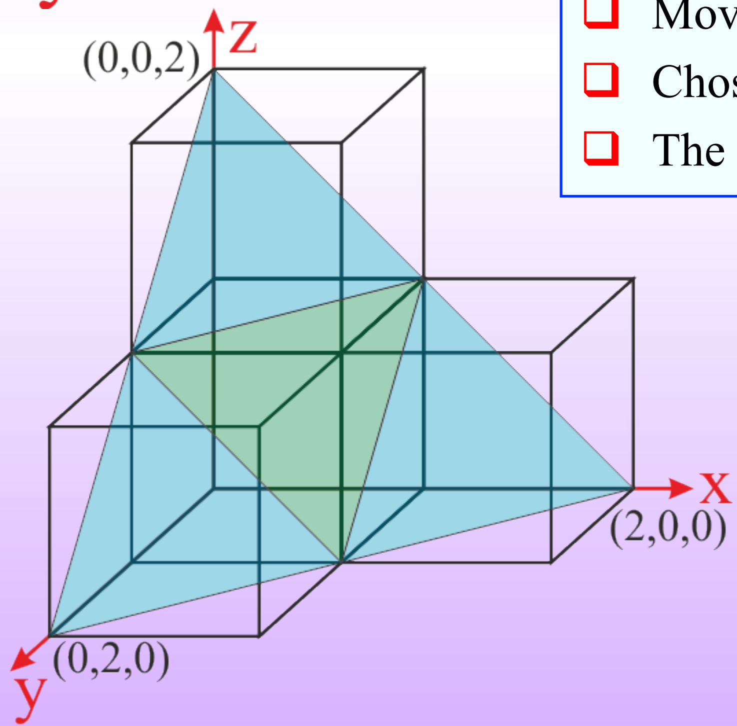


(Fig.3)

Q & A

What are the Miller indices of the green plane in the figure below?





- Extend the plane to intersect the x,y,z axes.
- The intercepts are: 2,2,2
- Reciprocal: ½, ½, ½
- Smallest ratio: 1,1,1
- Enclose in brackets to get Miller indices: (111)

- Another method.
- Move origin (‘O’) to opposite vertex (of the cube).
- Chose new axes as: -x, -y, -z.
- The new intercepts will be: 1,1,1

Multiplicity factor

This concept is very useful in X-Ray Diffraction

Advanced Topic

Cubic	hkl	hhl	hk0	hh0	hhh	h00	
	48*	24	24*	12	8	6	
Hexagonal	hk.l	hh.l	h0.l	hk.0	hh.0	h0.0	00.l
	24*	12*	12*	12*	6	6	2
Tetragonal	hkl	hhl	h0l	hk0	hh0	h00	00l
	16*	8	8	8*	4	4	2
Orthorhombic	hkl	hk0	h0l	0kl	h00	0k0	00l
	8	4	4	4	2	2	2
Monoclinic	hkl	h0l	0k0				
	4	2	2				
Triclinic	hkl						
	2						

* Altered in crystals with lower symmetry *(of the same crystal class)*