Analytical Methods for Materials

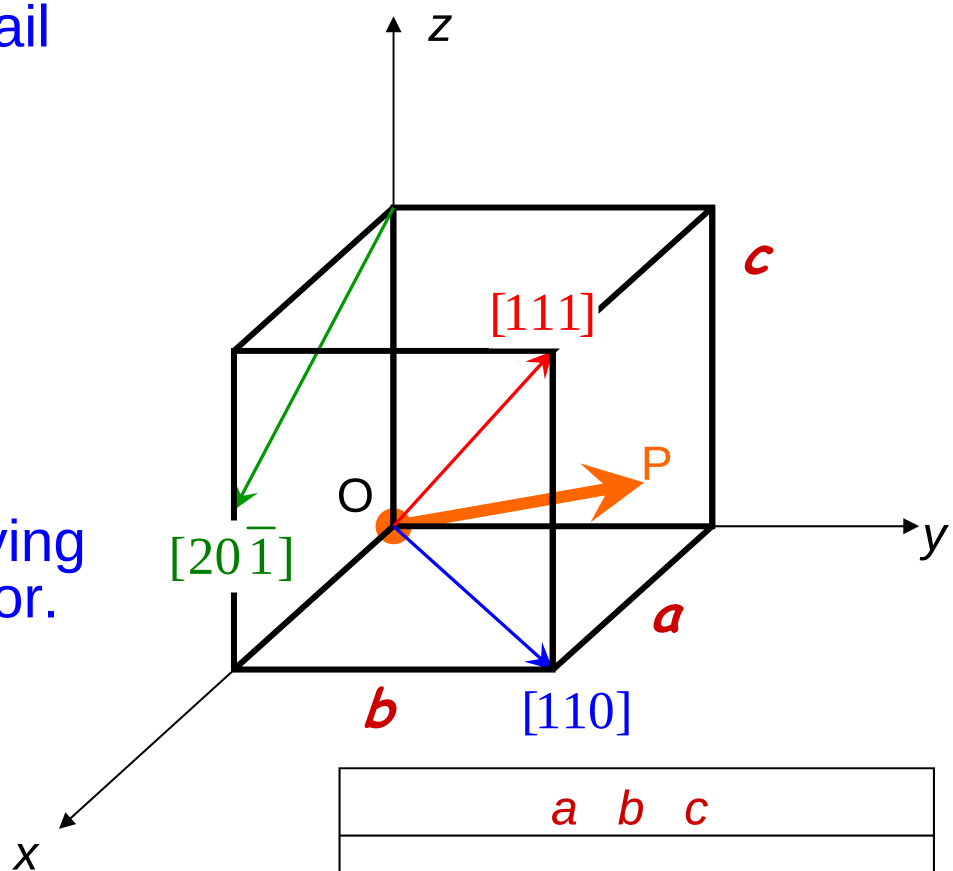
Lesson 8
Lattice Planes and Directions

Suggested Reading

- Chapters 2 and 6 in Waseda

Directions and Miller Indices

- *Draw vector* and define the tail as the origin.
- *Determine the length of the vector projection* in unit cell dimensions
  - *a*, *b*, and *c*.
- *Remove fractions* by multiplying by the smallest possible factor.
- *Enclose* in square brackets
- Negative indices are written with a bar over the number..

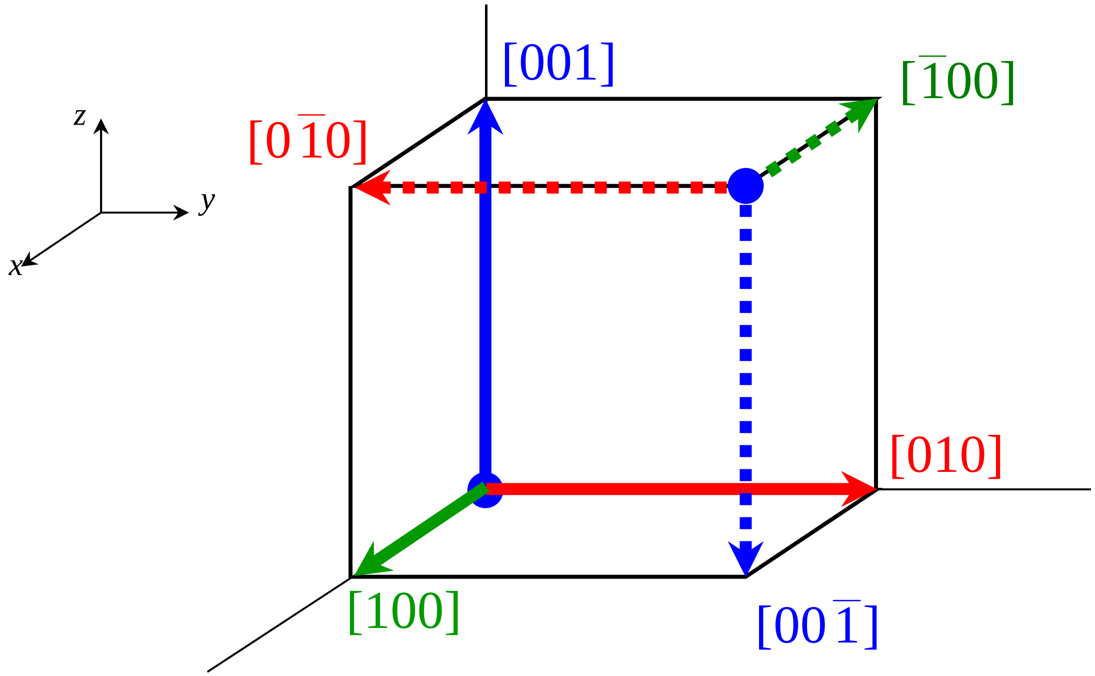


a b c

Families of Directions

(i.e., directions of a form)

- In cubic systems, directions that have the same indices are equivalent regardless of their order or sign.



The family of <100> directions is:

[100], $[\bar{1}00]$

[010], $[0\bar{1}0]$

[001], $[00\bar{1}]$

We enclose indices in carats rather than brackets to indicate a family of directions

All of these vectors have the same "size" and # lattice points/length

<100>

CUBIC <*aaa*>

$[100]$ $[010]$ $[001]$

$[\bar{1}00]$ $[0\bar{1}0]$ $[00\bar{1}]$

TETRAGONAL <*aac*>

$[100]$ $[010]$

$[\bar{1}00]$ $[0\bar{1}0]$

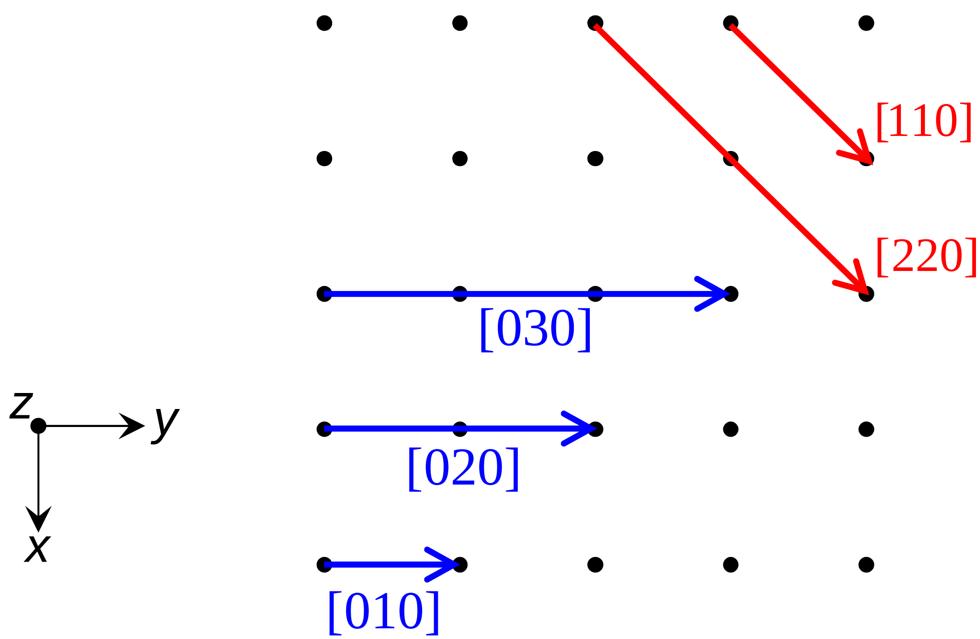
ORTHORHOMBIC <*abc*>

$[100]$ $[\bar{1}00]$

In non-cubic systems, directions with the same indices may not be equivalent.

Directions in Crystals

Directions and their multiples are identical



Ex.:

$[220] = 2 \times [110]$

Vectors and multiples of vectors have the same # lattice points/length

Miller Indices for Planes

★ Specific crystallographic plane: (*hkl*)

★ Family of crystallographic planes: {*hkl*}

– Ex.: (*hkl*), (*lkh*), (*hlk*) … etc.

– In <u>cubic</u> systems, planes having the same indices are equivalent regardless of order or sign.

- In hexagonal crystals, we use a four index system ($h\ k\ i\ l$).
  - We can convert from three to four indices
    - $h+k = -i$

FAMILY OF PLANES

ALL MEMBERS HAVE SAME ARRANGEMENT OF LATTICE POINTS

$$\{h\ k\ l\}$$

We use Miller indices to denote planes

PROCEDURES FOR INDICES OF PLANES
(Miller indices)

1. ***Identify the coordinate intercepts*** of the plane (*i.e.*, the coordinates at which the plane intersects the x, y, and z axes).

   - If plane is parallel to an axis, the intercept is taken as infinity (∞).

   - If the plane passes through the origin, consider an equivalent plane in an adjacent unit cell or select a different origin for the same plane.

2. ***Take reciprocals*** of the intercepts.

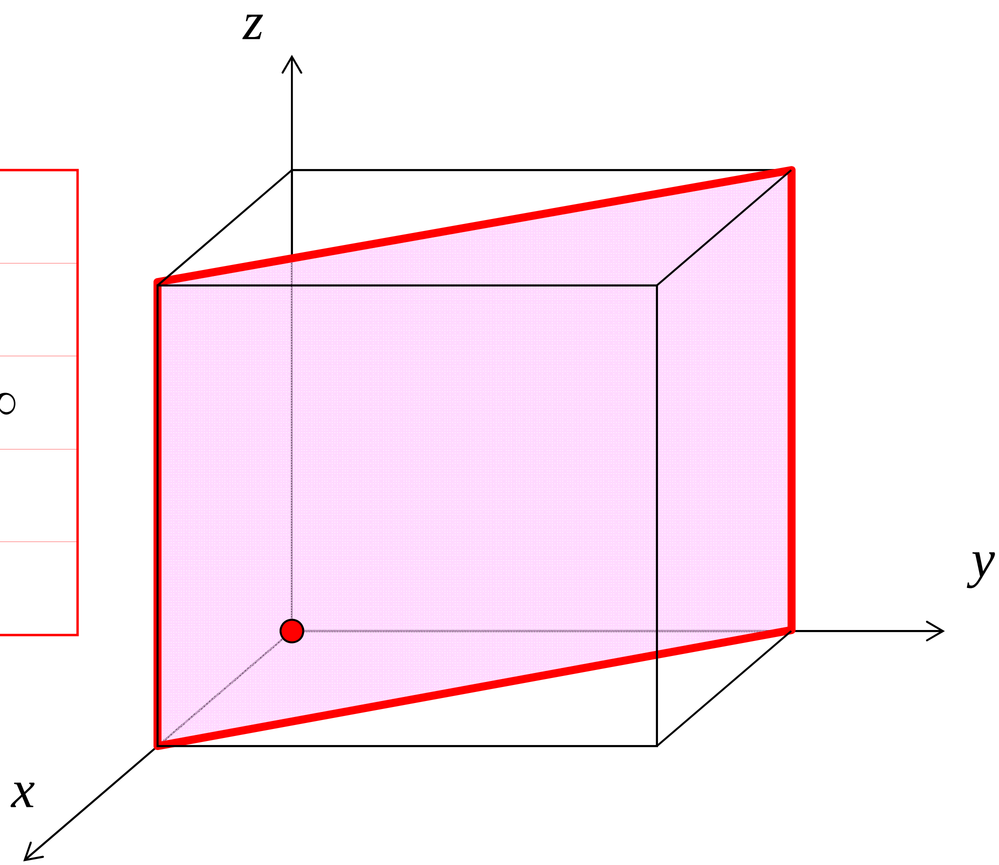
3. ***Clear fractions*** to the lowest integers.

4. ***Cite specific planes in parentheses***, ($h\ k\ l$), placing bars over negative indices.

MILLER INDICES FOR A SINGLE PLANE

	x	*y*	*z*
Intercept	1	1	∞
Reciprocal	1/1	1/1	$1/\infty$
Clear	1	1	0
INDICES	**1**	**1**	**0**

(110)



The {110} family of planes

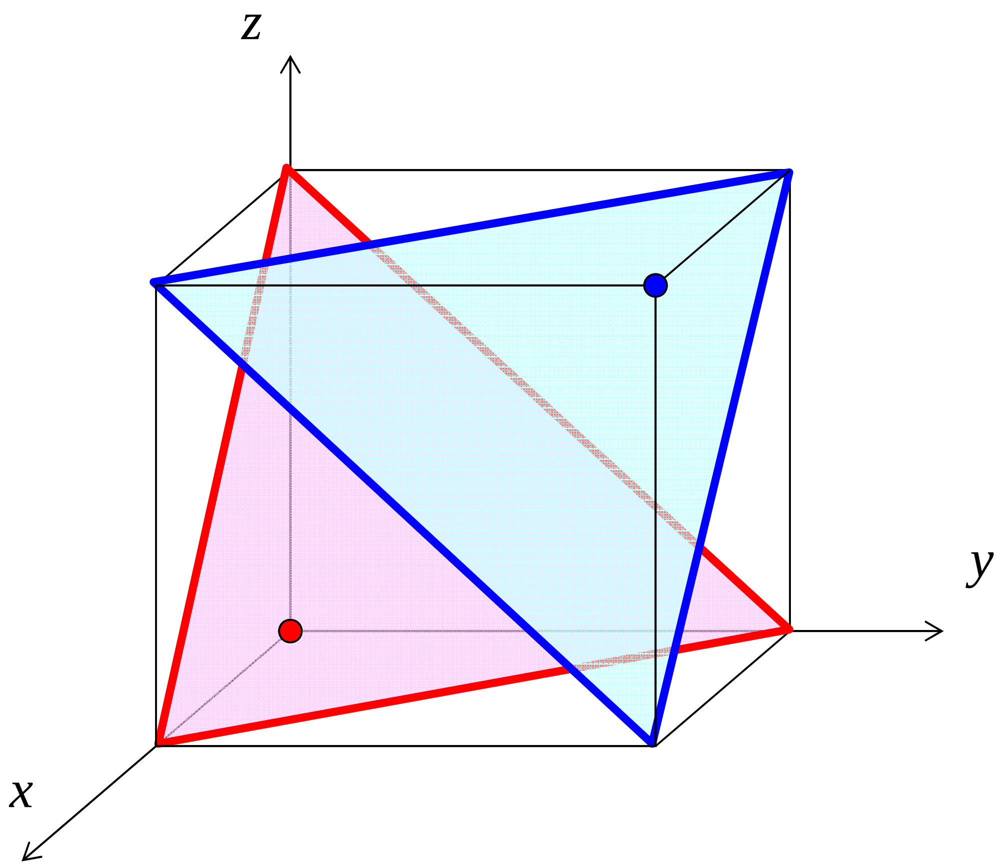
$(110), (011), (101), (\bar{1}\bar{1}0), (0\bar{1}\bar{1}), (\bar{1}0\bar{1})$

$(\bar{1}10), (1\bar{1}0), (\bar{1}01), (10\bar{1}), (01\bar{1}), (0\bar{1}1)$

MILLER INDICES FOR A SINGLE PLANE – cont'd

	x	**y**	**z**
Intercept	1	1	1
Reciprocal	1/1	1/1	1/1
Clear	1	1	1
INDICES	**1**	**1**	**1**

	x	**y**	**z**
Intercept	-1	-1	-1
Reciprocal	-1/1	-1/1	-1/1
Clear	-1	-1	-1
INDICES	$\bar{1}$	$\bar{1}$	$\bar{1}$

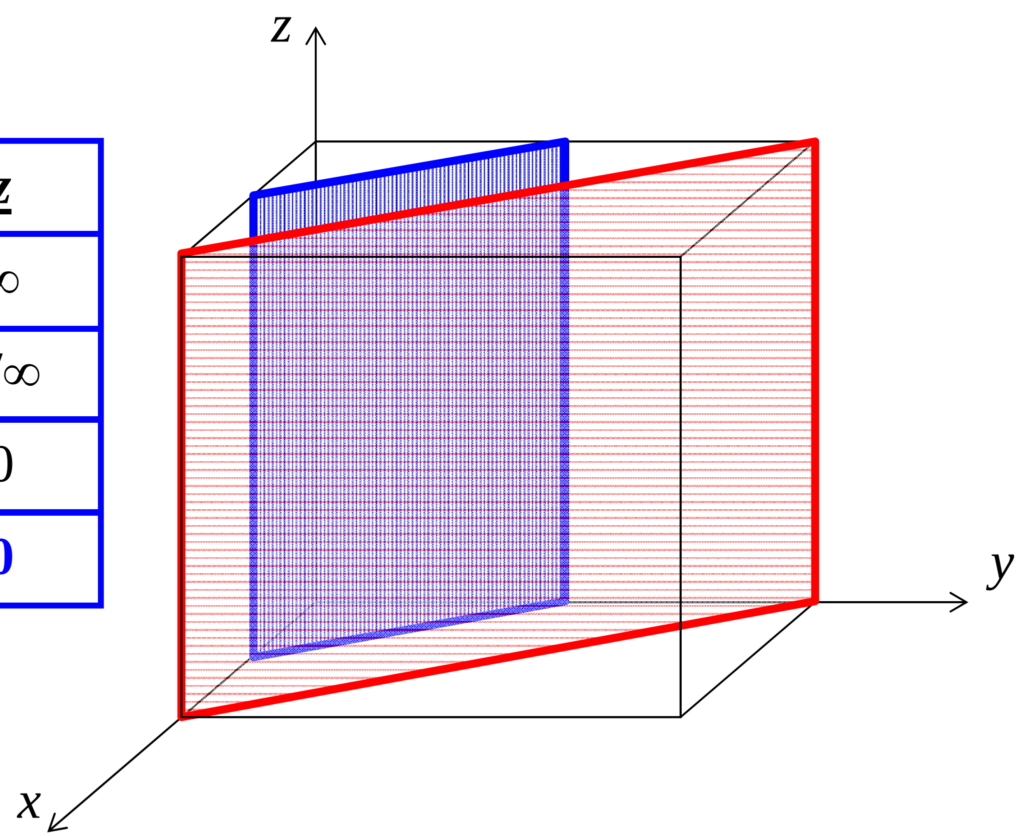


$$(111) = (\bar{1}\bar{1}\bar{1})$$

MILLER INDICES FOR A SINGLE PLANE - cont'd

	x	*y*	*z*
Intercept	1/2	1/2	∞
Reciprocal	2/1	2/1	1/∞
Clear	2	2	0
INDICES	**2**	**2**	**0**

(220)



Planes and their multiples are not identical

(220) ≠ (110)

Planes in Unit Cells

Some important aspects of Miller indices for planes:

1. *Planes and their negatives are identical*.
   This was NOT the case for directions.

2. *Planes and their multiples are **NOT** identical*.
   This is opposite to the case for directions.

3. In *cubic systems*, a *direction* that has the *same indices as a plane is $\perp$ to that plane*.
   This is not always true for non-cubic systems.

Table 2.2 Multiplicity factors for crystalline powder samples

Cubic		hkl	hkk	$hk0$	$hh0$	hhh	$h00$		
		48*	24	24*	12	8	6		
Hexagonal		$hk \cdot l$	$hh \cdot l$	$h0 \cdot l$	$hk \cdot 0$	$hh \cdot 0$	$h0 \cdot 0$	$00 \cdot l$	
		24*	12	12	12*	6	6	2	
Trigonal	Referred to	hkl	$\bar{k}kh$	hkk	$hk0$	$\bar{k}hh$	hhh	$hh0$	$h00$
	rhombohedral axes	12*	12*	6	12*	6	2	6	6
	Referred to	$hk \cdot l$	$hh \cdot l$	$h0 \cdot l$	$hk \cdot 0$	$hh \cdot 0$	$0h \cdot 0$	$00 \cdot l$	
	hexagonal axes	12*	12*	6	12*	6	6	2	
Tetragonal		hkl	hhl	$hh0$	$hk0$	$h0l$	$h00$	$00l$	
		16*	8	4	8*	7	4	2	
Orthorhombic		hkl	$hk0$	$h00$	$0k0$	$00l$	$h0l$	$0kl$	
		8	4	2	2	2	4	4	
Monoclinic		hkl	$hk0$	$0kl$	$h0l$	$h00$	$0k0$	$00l$	
(Orthogonal axis: b)		4	4	4	2	2	2	2	
Triclinic		hkl	$hk0$	$0kl$	$h0l$	$h00$	$0k0$	$00l$	
		2	2	2	2	2	2	2	

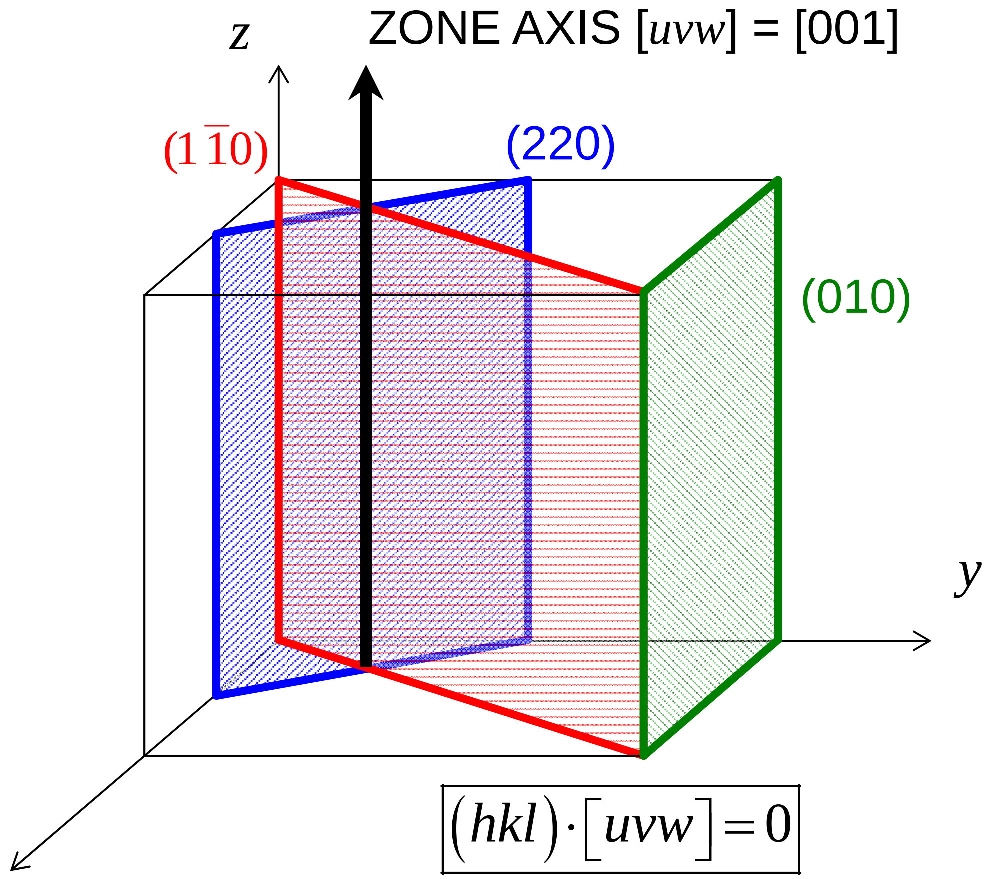
*In some crystals, planes having these indices comprise of two forms with the same spacing but different structure factor. In such case, the multiplicity factor for each form is half the value given here.

Planes of a Zone

- A <u>zone</u> is a <u>direction</u> [*uvw*]

- Planes belonging to a particular zone share a direction.

  This direction is known as a <u>zone axis</u>.



$$\boxed{(hkl)\cdot[uvw]=0}$$

$$(1\bar{1}0)\cdot[001]=(1)(0)+(-1)(0)+(0)(1)=0$$

$$\therefore [001] \text{ lies on } (1\bar{1}0)$$

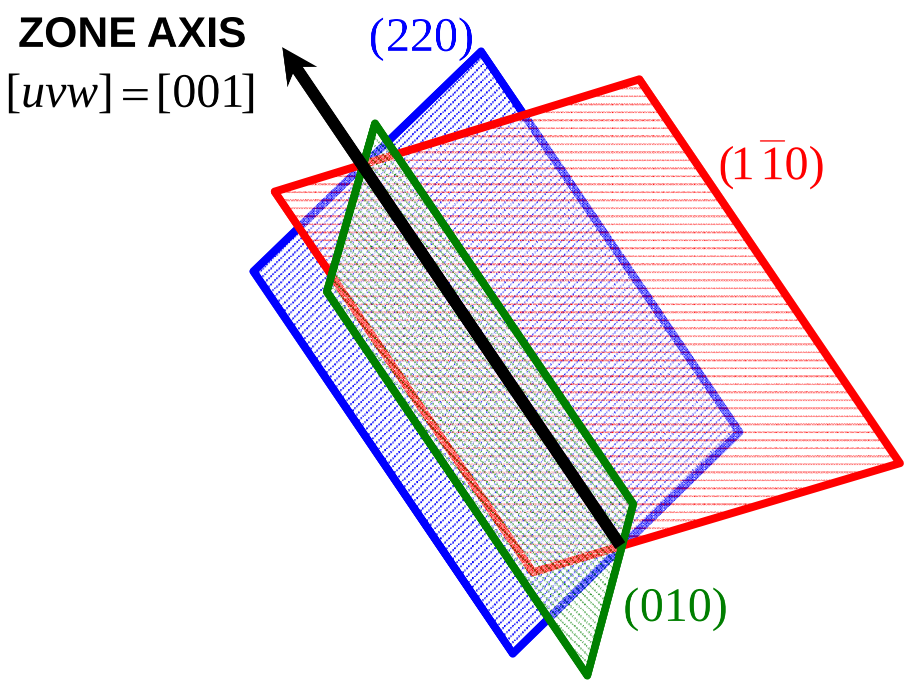
$$(220)\cdot[001]=(2)(0)+(2)(0)+(0)(1)=0$$

$$\therefore [001] \text{ lies on } (220)$$

Weiss Zone Law

- If a direction $[uvw]$ lies in a plane $\{hkl\}$:

$$[uvw]\cdot\{hkl\} = uh + vk + wl = 0$$

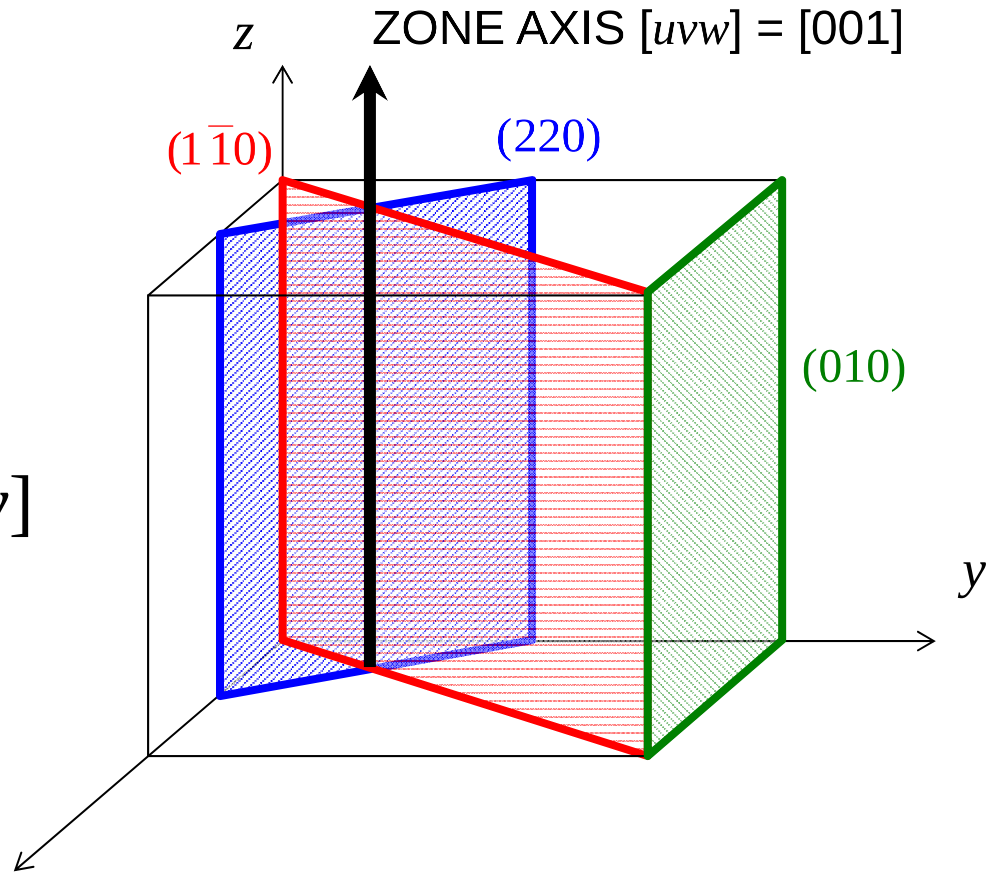


This rule holds for <u>all</u> crystal systems

How to Determine the Zone Axis

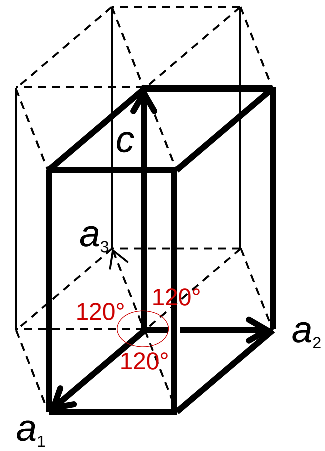
- Take the cross product of the intersecting planes.

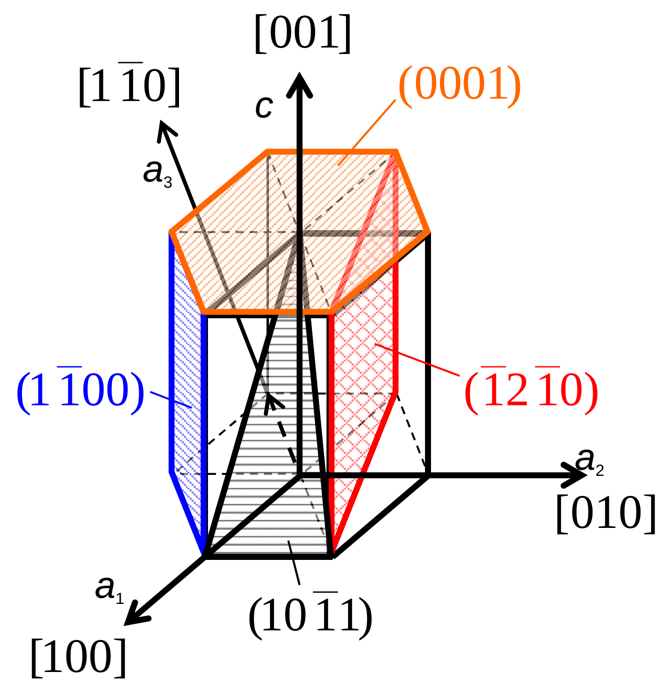
$$(h_1k_1l_1) \times (h_2k_2l_2) = [uvw]$$



Indexing in Hexagonal Systems

- The regular 3 index system is not suitable.
- Planes with the same indices do not necessarily look like.
- 4 index system introduced.
  - Miller-Bravais indices





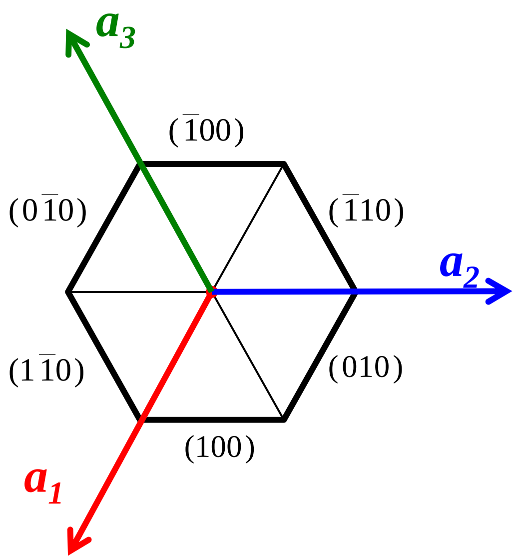
Indexing in Hexagonal Systems

- Planes:
  - (hkl) becomes ($hkil$)
  - $i = -(h+k)$
- Directions:
  - [UVW] becomes [$uvtw$]
  - $U = u\text{-}t$; $u = (2U - V)/3$
  - $V = v\text{-}t$; $v = (2V - U)/3$
  - $W=w$; $t=-(U+V)$

PLANES

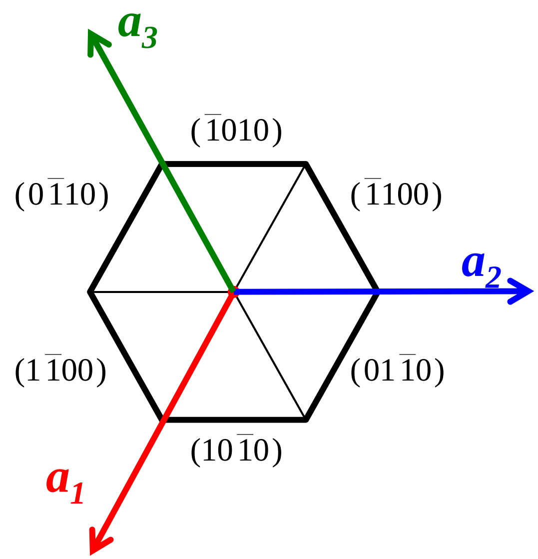
Miller Indices

(hkl)



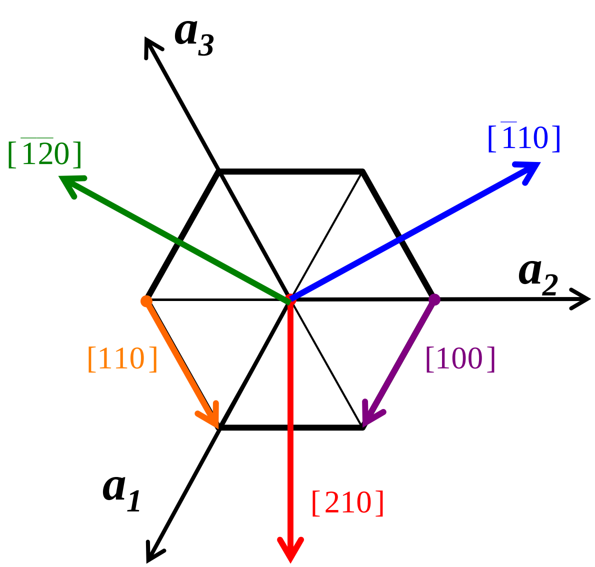
Miller-Bravais Indices

(hkil)

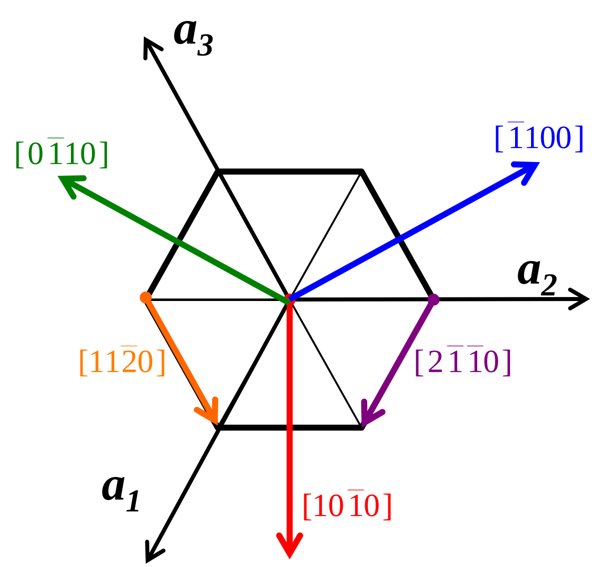


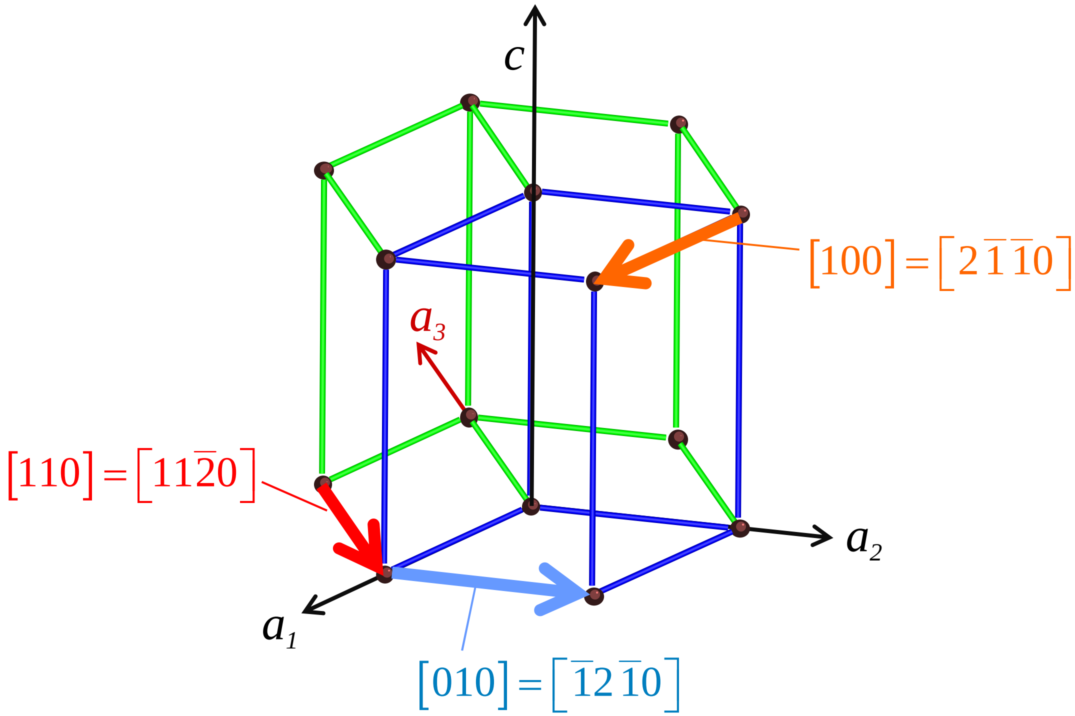
DIRECTIONS

(UVW)



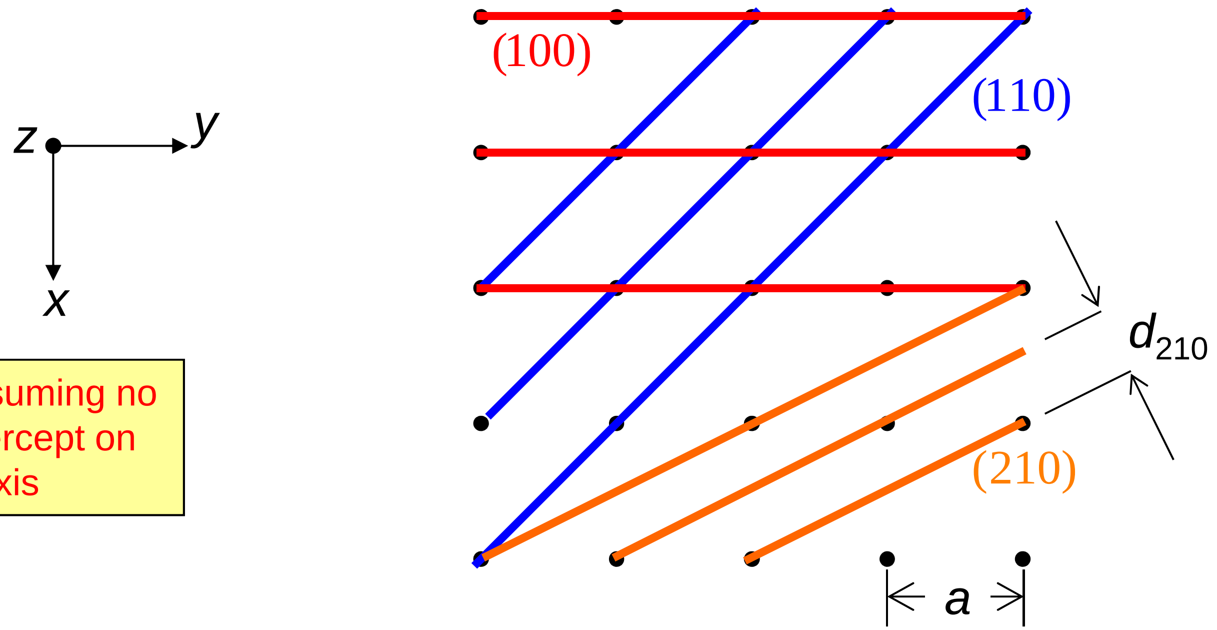
(uvtw)





Some typical directions in an HCP unit cell using three- and four-axis systems.

Inter-planar Spacings



Assuming no intercept on *z*-axis

- The inter-planar spacing in a particular direction is the distance between equivalent planes of atoms.

★ ***Each material has a set of characteristic inter-planar spacings.*** They are directly related to crystal size (i.e. lattice parameters) and atom location.

Interplanar Spacing – cont’d

CUBIC: $$\frac{1}{d^2} = \frac{h^2 + k^2 + l^2}{a^2}$$

HEXAGONAL: $$\frac{1}{d^2} = \frac{4}{3}\left(\frac{h^2 + hk + k^2}{a^2}\right) + \frac{l^2}{c^2}$$

TETRAGONAL: $$\frac{1}{d^2} = \frac{h^2 + k^2}{a^2} + \frac{l^2}{c^2}$$

RHOMBOHEDRAL: $$\frac{1}{d^2} = \frac{\left(h^2 + hk + k^2\right)\sin^2\alpha + 2\left(hk + kl + hl\right)\left(\cos^2\alpha - \cos\alpha\right)}{a^2\left(1 - 3\cos^2\alpha + 2\cos^3\alpha\right)}$$

ORTHORHOMBIC: $$\frac{1}{d^2} = \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}$$

MONOCLINIC: $$\frac{1}{d^2} = \frac{1}{\sin^2\beta}\left(\frac{h^2}{a^2} + \frac{k^2\sin^2\beta}{b^2} + \frac{l^2}{c^2} - \frac{2hl\cos\beta}{ac}\right)$$

TRICLINIC*: $$\frac{1}{d^2} = \frac{1}{V^2}\left(S_{11}h^2 + S_{22}k^2 + S_3 l^2 + 2S_{12}hk + 2S_{23}kl + 2S_{13}hl\right)$$

$$S_{11} = b^2c^2\sin^2\alpha \;;\; S_{22} = a^2c^2\sin^2\beta \;;\; S_{33} = a^2b^2\sin^2\gamma$$

$$S_{12} = abc^2\left(\cos\alpha\cos\beta - \cos\gamma\right) \;;\; S_{23} = a^2bc\left(\cos\beta\cos\gamma - \cos\alpha\right) \;;\; S_{13} = ab^2c\left(\cos\gamma\cos\alpha - \cos\beta\right)$$

$$V = abc\sqrt{1 - \cos^2\alpha - \cos^2\beta - \cos^2\gamma + 2\cos\alpha\cos\beta\cos\gamma}$$