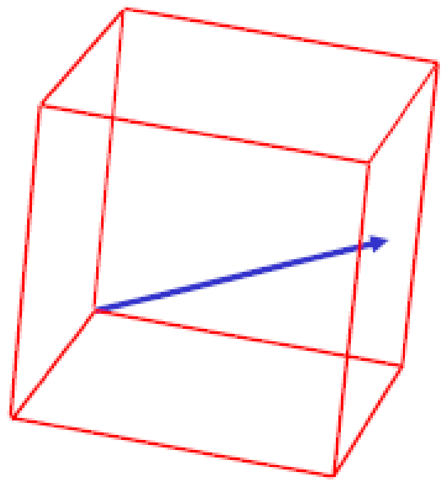
<u>**Crystallographic Directions, and Planes**</u>

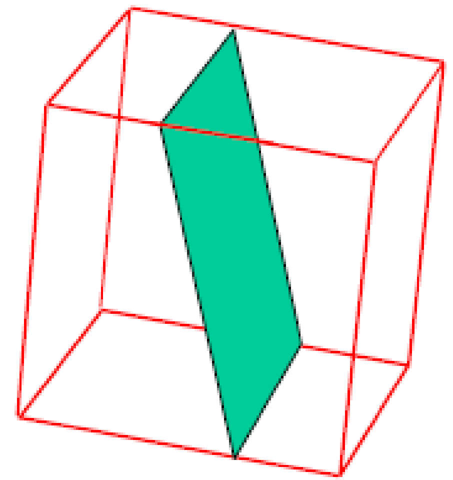
Now that we know how atoms arrange themselves to form crystals, *we need a way to identify directions and planes of atoms.*

<u>Why?</u>

- Deformation under loading occurs on certain crystalline planes and in certain crystallographic directions. Before we can predict how materials fail, we need to know what modes of failure are more likely to occur.
- Other properties of materials (*electrical conductivity, thermal conductivity, elastic modulus*) can vary in a crystal with orientation.



direction



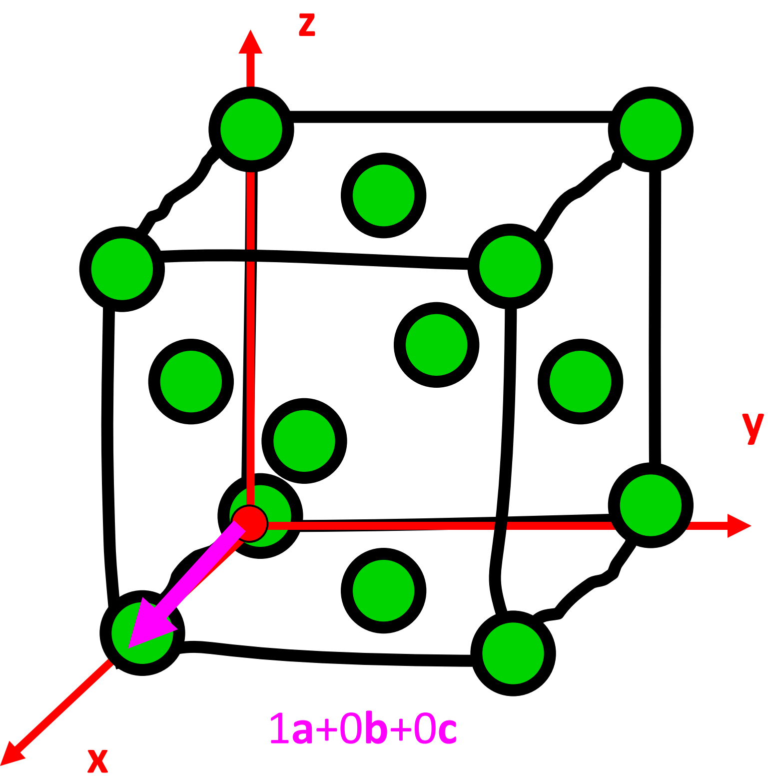
plane

- It is often necessary to be able to specify certain directions and planes in crystals.
- Many material properties and processes vary with direction in the crystal.
- Directions and planes are described using three integers - Miller Indices

Miller Indices of Directions

1. Choose a point **on the direction** as the origin.

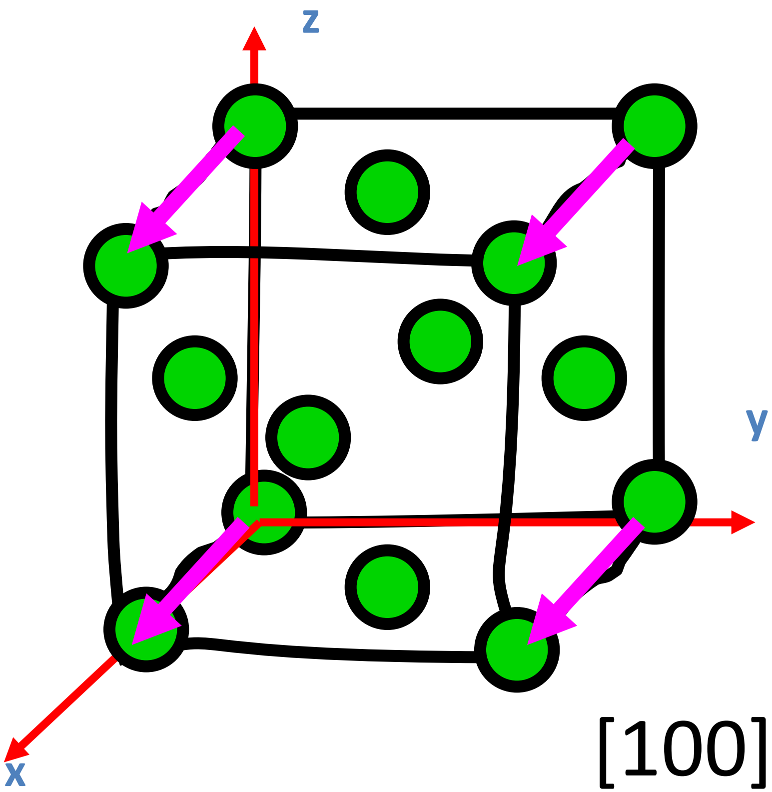
2. Choose a coordinate system with axes parallel to the unit cell edges.



3. Find the coordinates of another point on the direction in terms of **a**, **b** and **c** **1, 0, 0**

4. Reduce the coordinates to smallest integers. **1, 0, 0**

5. Put in square brackets **[100]**



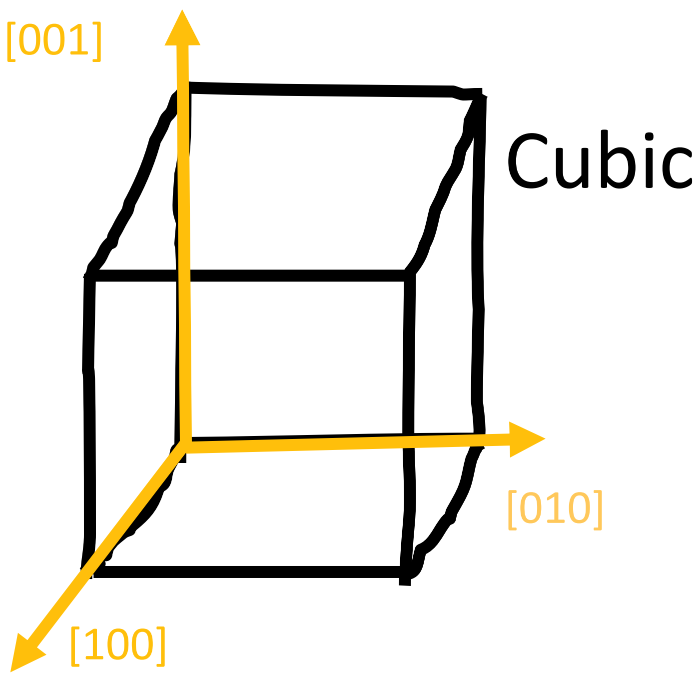
[100]

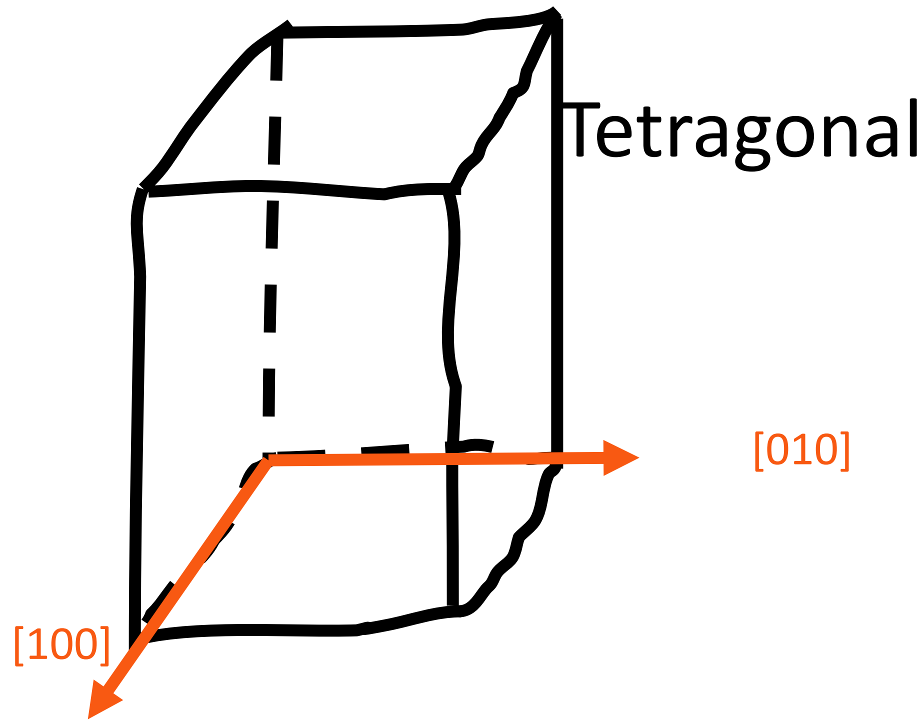
Miller indices of a direction represents only the orientation of the line corresponding to the direction and not its position or sense

All parallel directions have the same Miller indices

Miller indices of a family of symmetry related directions

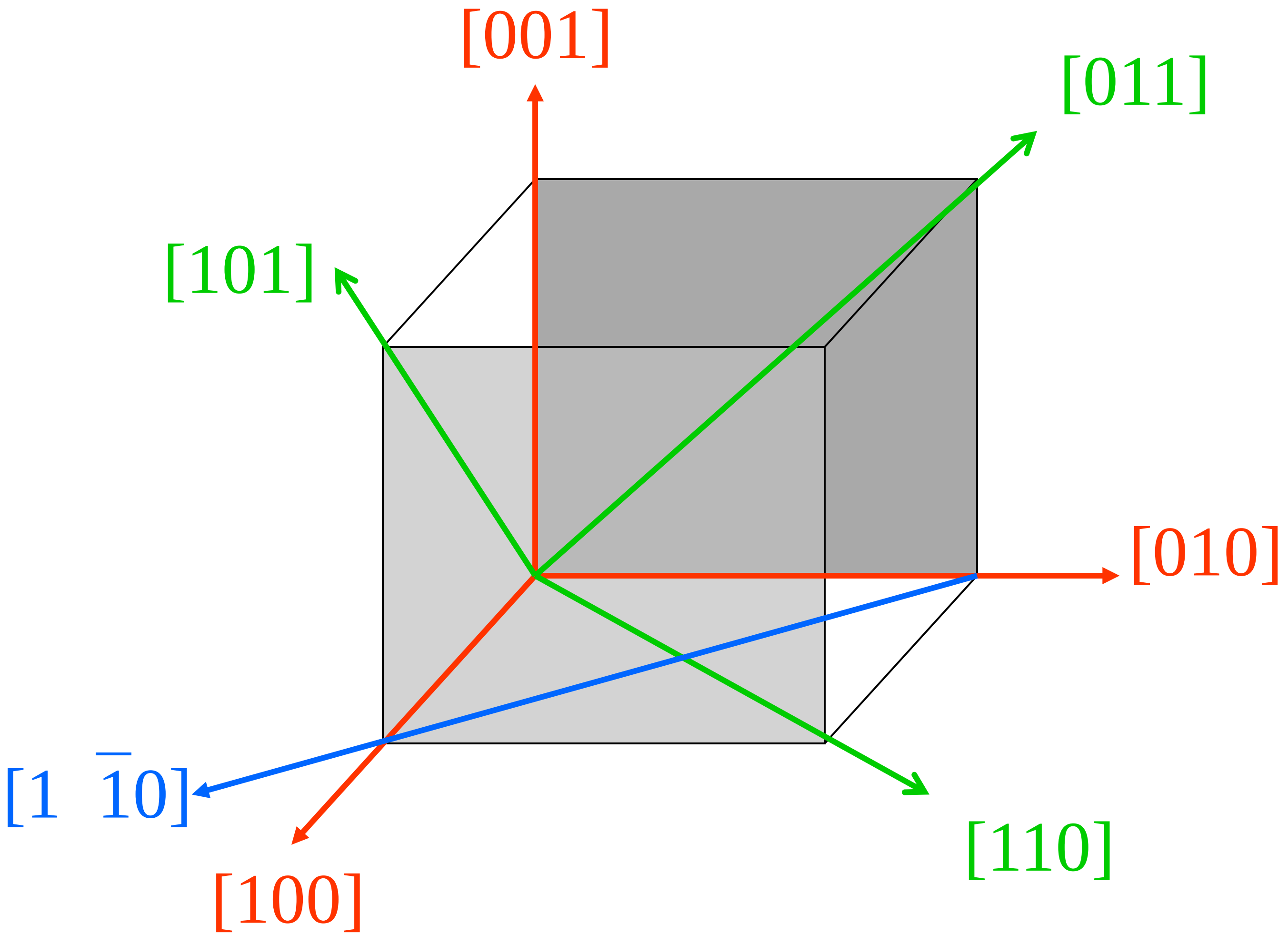
$\langle uvw \rangle$ **= [uvw] and all other directions related to [uvw] by the symmetry of the crystal**





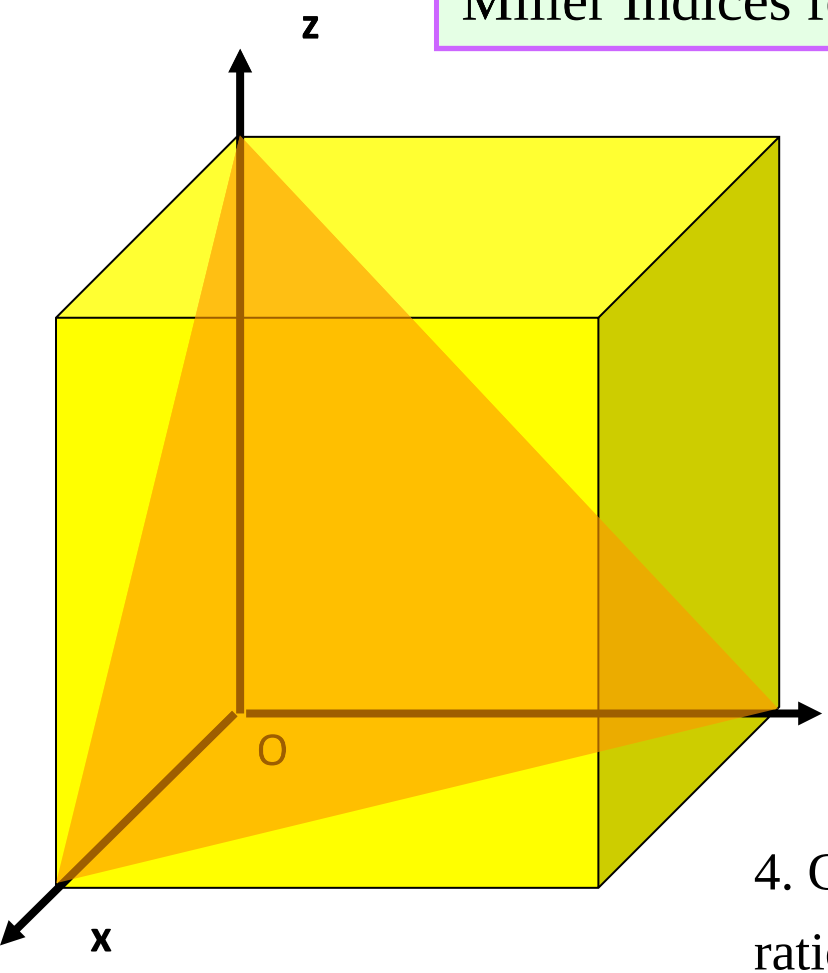
$\langle 100 \rangle_{cubic}$ = [100], [010], [001]

$\langle 100 \rangle_{tetragonal}$ = [100], [010]



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

Miller Indices for planes



1. Select a crystallographic coordinate system with **origin not on the plane**

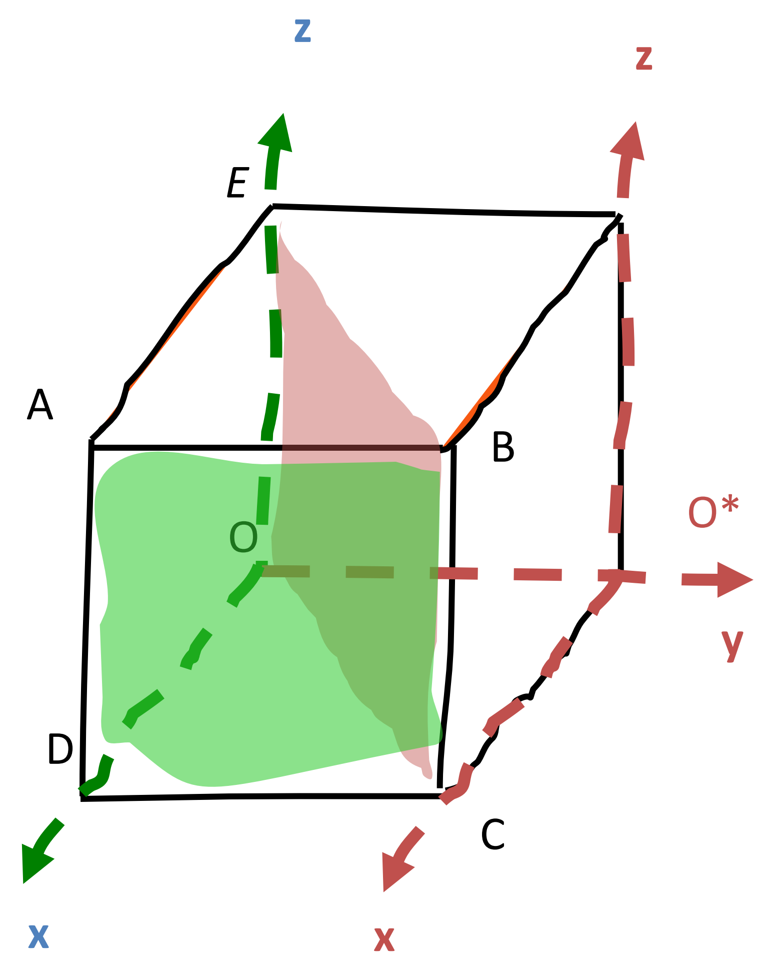
2. Find intercepts along axes in terms of respective lattice parameters **1 1 1**

3. Take reciprocal **1 1 1**

4. Convert to smallest integers in the same ratio **1 1 1**

5. Enclose in parenthesis **(111)**

Miller Indices for planes (contd.)

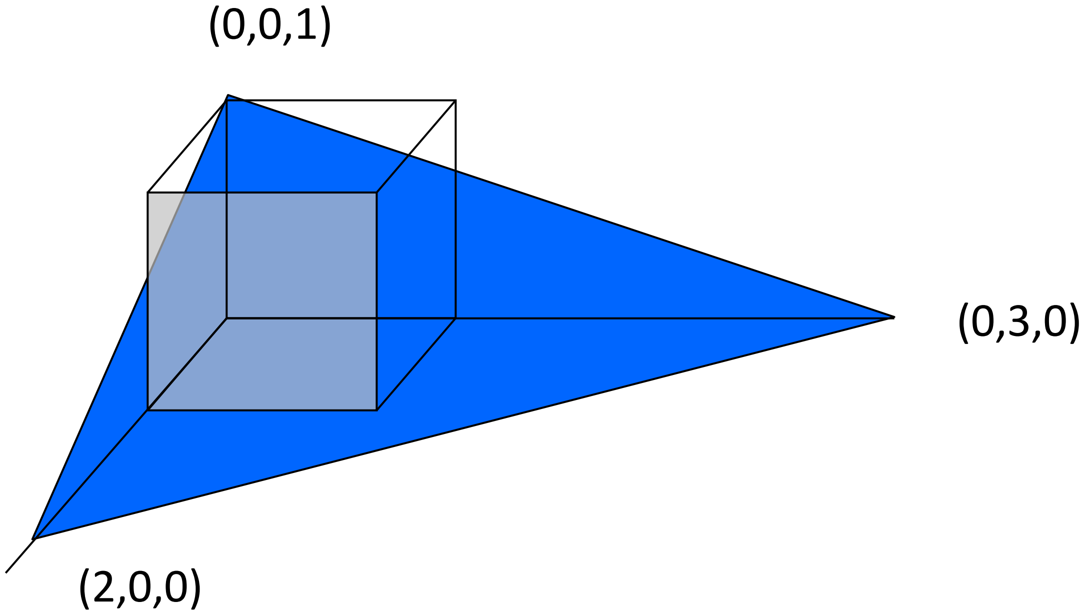


Plane	ABCD	OCBE
origin	O	O*
intercepts	$1\ \infty\ \infty$	$1\ {-1}\ \infty$
reciprocals	1 0 0	1 -1 0
Miller Indices	(1 0 0)	$(1\,\bar{1}\,0)$

Zero represents that the plane is parallel to the corresponding axis

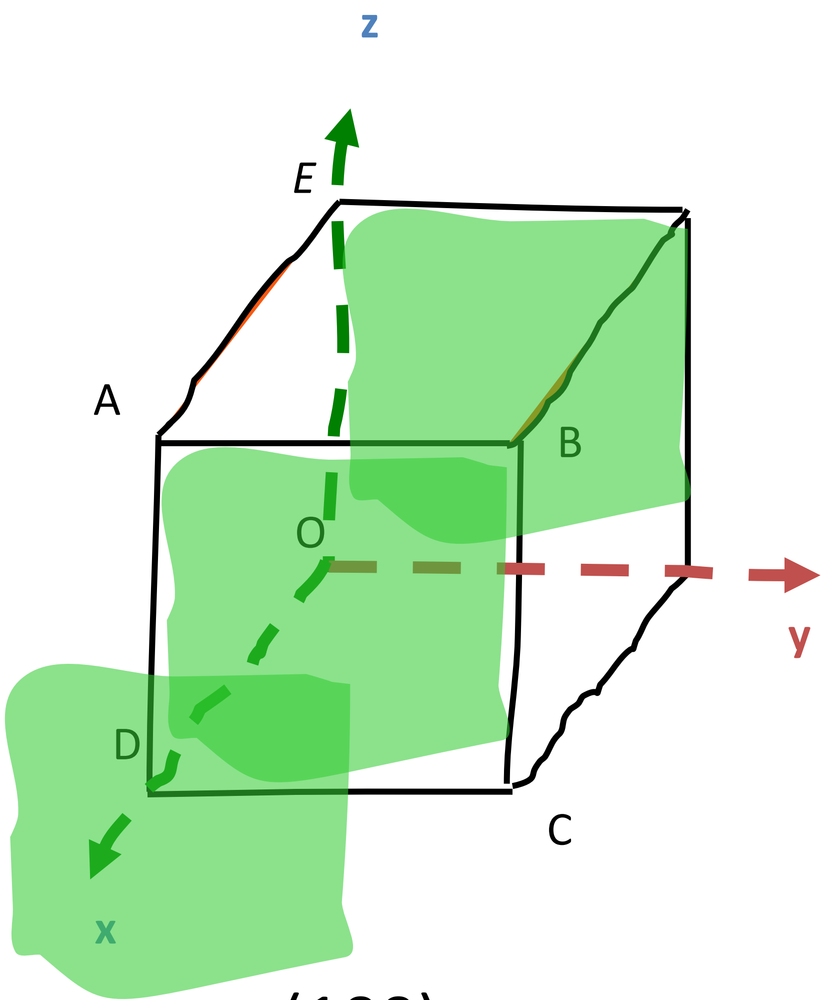
Bar represents a negative intercept

Miller Indices for planes



- 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)

Miller indices of a plane
specifies only its orientation in space not its position



(100)

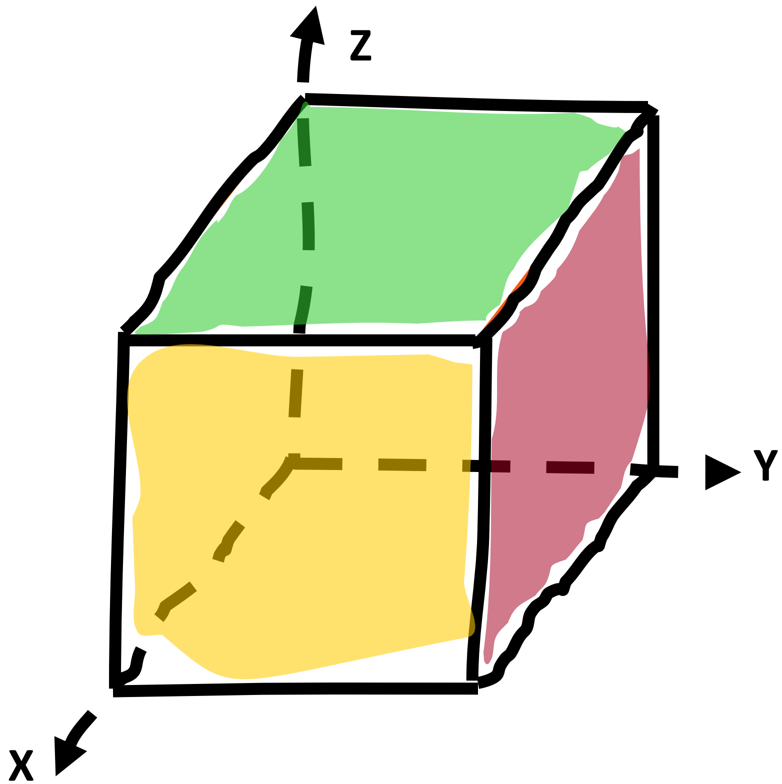
All parallel planes have the same Miller Indices

$$(h\ k\ l) \equiv (\bar{h}\ \bar{k}\ \bar{l})$$

$$(100) \equiv (\bar{1}00)$$

Miller indices of a family of symmetry related planes

$\{hkl\}$ = **(*hkl*) and all other planes related to (*hkl*) by the symmetry of the crystal**



All the faces of the cube are equivalent to each other by symmetry

Front & back faces: (100)

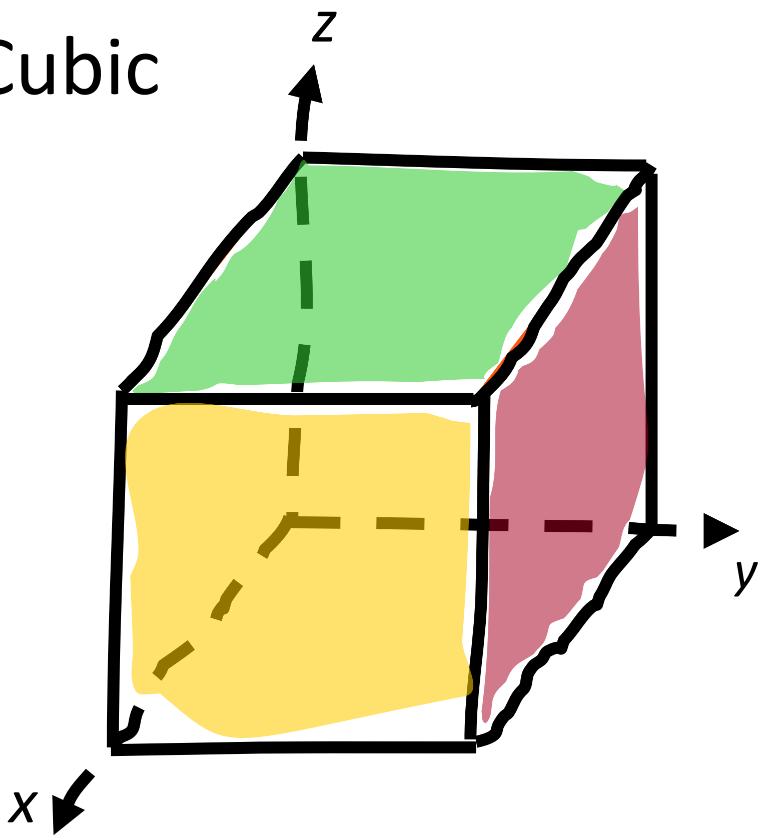
Left and right faces: (010)

Top and bottom faces: (001)

$$\{100\} = (100), (010), (001)$$

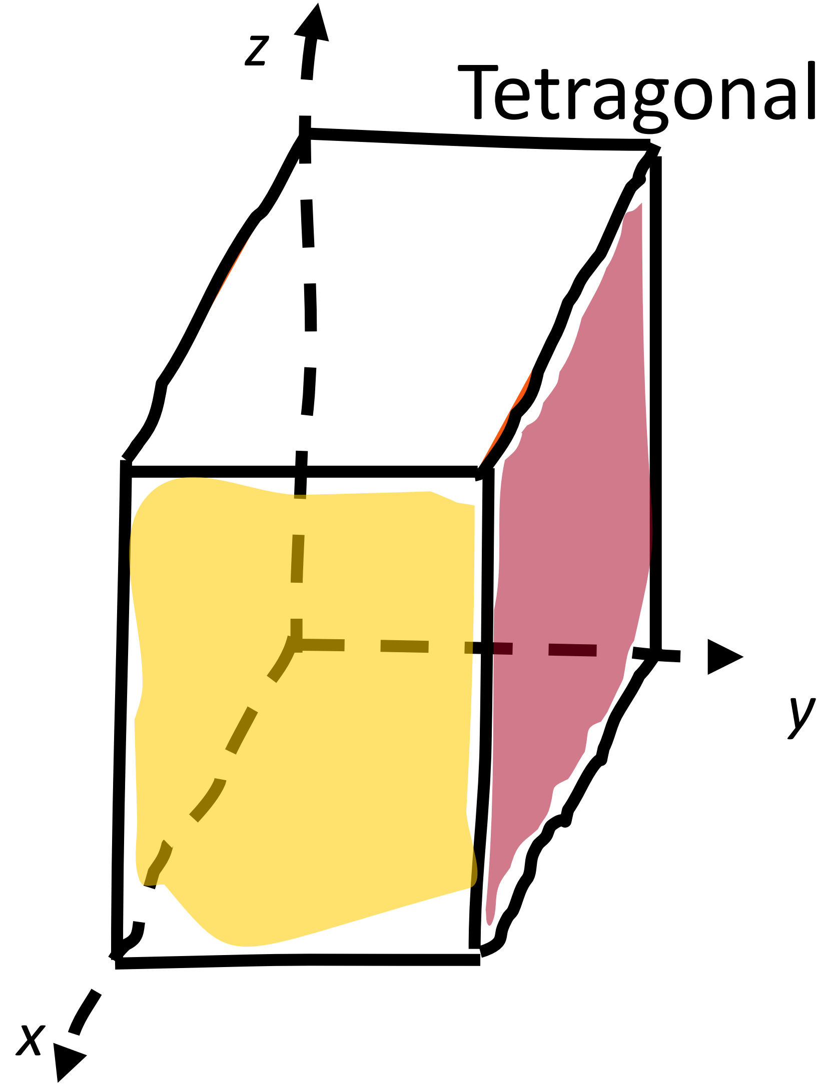
Miller indices of a family of symmetry related planes

Cubic



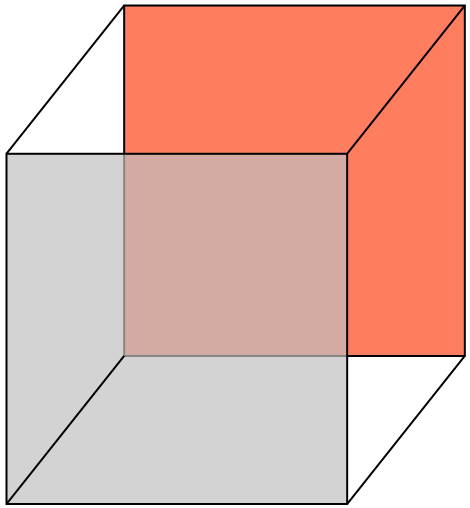
$\{100\}_{cubic}$ = (100), (010), (001)

Tetragonal



$\{100\}_{tetragonal}$ = (100), (010)

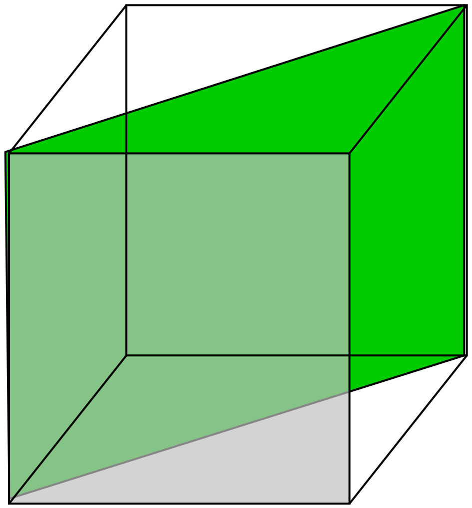
~~(001)~~



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

Plane $\rightarrow (100)$

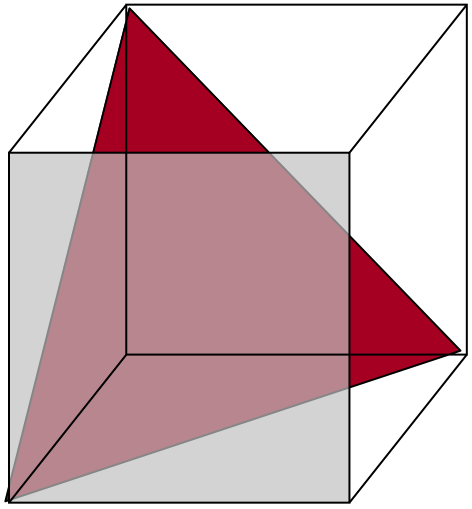
Family $\rightarrow \{100\} \rightarrow 3$



Intercepts $\rightarrow 1\ 1\ \infty$

Plane $\rightarrow (110)$

Family $\rightarrow \{110\} \rightarrow 6$



Intercepts $\rightarrow 1\ 1\ 1$

Plane $\rightarrow (111)$

Family $\rightarrow \{111\} \rightarrow 8$

(Octahedral plane)

Weiss zone law

Condition for a direction [*uvw*] to be parallel to a plane or lie in the plane (*hkl*):

$$\boxed{hu + kv + lw = 0}$$

True for ALL crystal systems

The Weiss zone law states that:

If the direction [*UVW*] lies in the plane (*hkl*), then:

$\boldsymbol{hU + kV + lW = 0}$

In a cubic system this is exactly analogous to taking the scalar product of the direction and the plane normal, so that if they are perpendicular, the angle between them, θ, is 90° , then cosθ = 0, and the direction lies in the plane. Indeed, in a **cubic** system, the scalar product can be used to determine the angle between a direction and a plane.

However, the Weiss zone law is more general, and can be shown to work for all crystal systems, to determine if a direction lies in a plane.

From the Weiss zone law the following rule can be derived:

The direction, [*UVW*], of the intersection of $(h_1k_1l_1)$ and $(h_2k_2l_2)$ is given by:

$\boldsymbol{U = k_1l_2 - k_2l_1}$

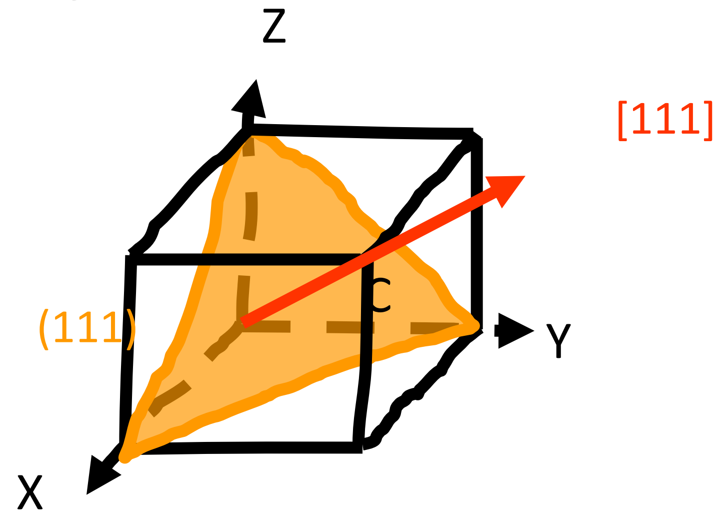
$\boldsymbol{V = l_1h_2 - l_2h_1}$

$\boldsymbol{W = h_1k_2 - h_2k_1}$

As it is derived from the Weiss zone law, this relation applies to all crystal systems, including those that are not orthogonal.

CUBIC CRYSTALS

$$[hkl] \perp (hkl)$$



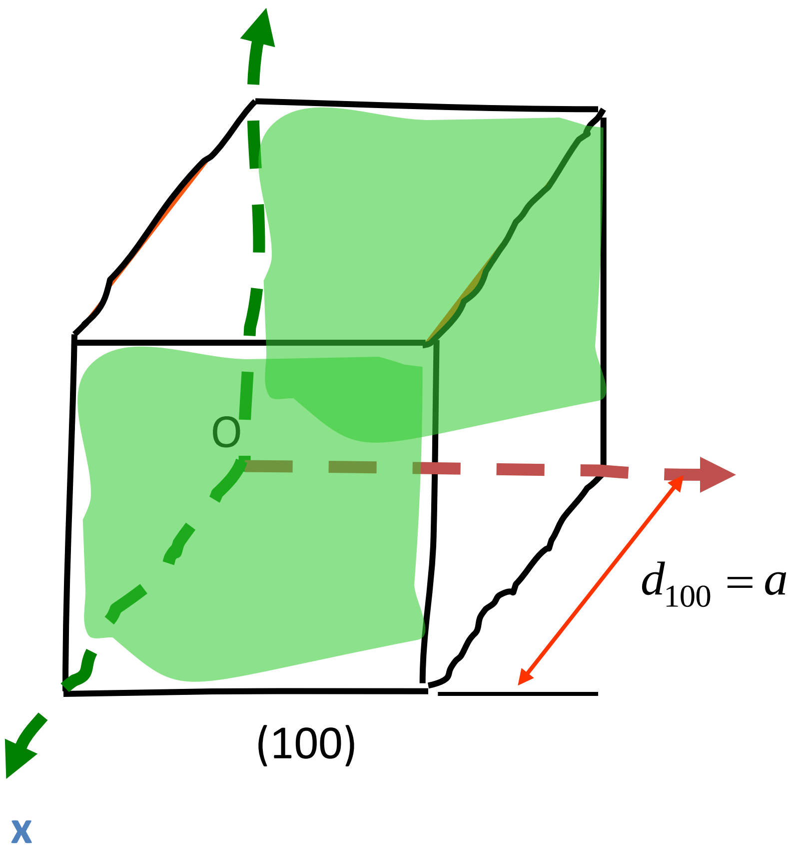
Angle between two directions $[h_1k_1l_1]$ and $[h_2k_2l_2]$:

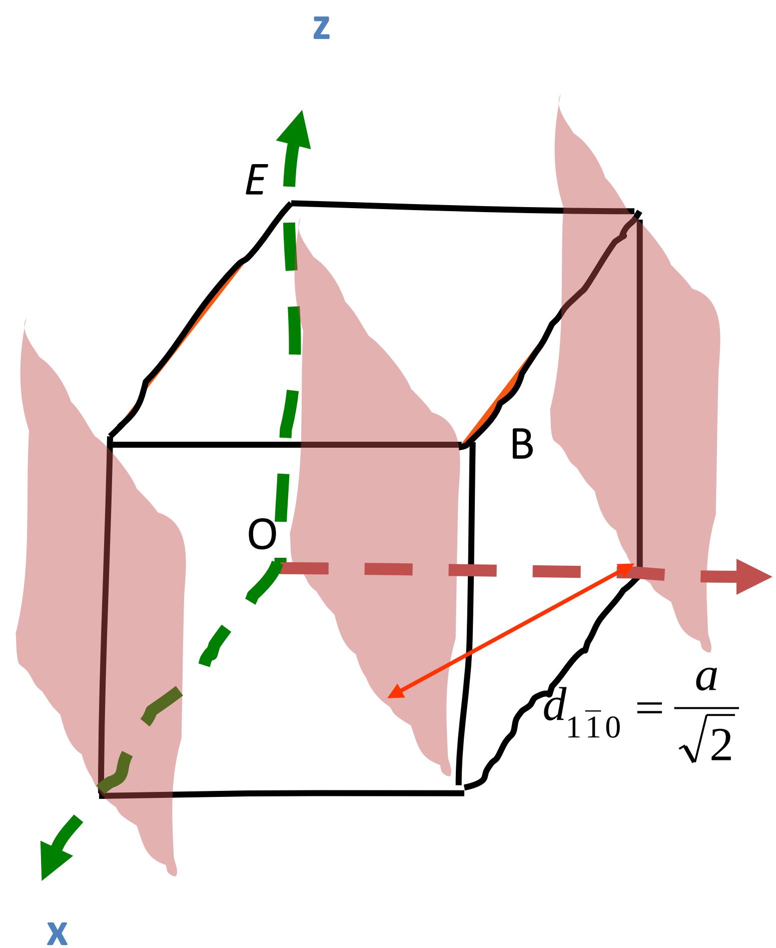
$$\cos\theta = \frac{h_1h_2 + k_1k_2 + l_1l_2}{\sqrt{h_1^2 + k_1^2 + l_1^2}\sqrt{h_2^2 + k_2^2 + l_2^2}}$$

d_{hkl}

Interplanar spacing between 'successive' (hkl) planes passing through the **corners** of the unit cell

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





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