State of Matter

- Solid
- Fluid
    - Liquid
    - Gas

Properties of Solid

1. Incompressible
    - Closely packed atom/molecule
    - Interatomic distance is very less.
2. Inflexible
3. Have mechanical strength
4. Have specific shape

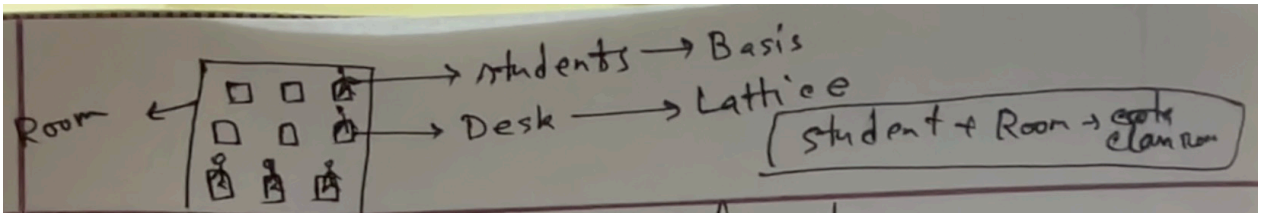
Types of Solid

Broadly 3 types of sold found in nature.

1. Crystalline solid
2. Poly-crystalline solid
3. Non-crystalline solid

Crystalline Solid

- **Structure :** The constituents(atoms, molecules or ions) are arranged in an orderly manner in a definite geometric shape.
  - Regular arrangement of constituent atom
  - Definite regular geometry



- Long range order
- **Lattice :** Regular and periodic arrangement of points in space.

- **Basis :** Atom or group of atoms.

$$Lattice + Basis = Crystal\ Struct.$$

- **Example ----->** Dimond salt, most of the metals.

Poly-crystalline Solid

A **polycrystalline solid** is a material made up of many small crystals or **grains**, each with its own **crystalline structure and orientation**, but joined together.

- Occur as powder resemble amorphous but properties are just like crystalline solid.
- Arrangement amorphous
- Looks like amorphous
- Properties like crystalline crystalline
- **Example --->** Sand, Ceramic

Non-crystalline / Amorphous

- Constituents (atoms, ions or molecules) are not arranged in a regular manner.
  - No regular geometry
- Have no electrical conductivity
- Melting point is not fixed
- **Example --->** Glass, Rubber

Difference Between Crystalline & Non-crystalline Solid

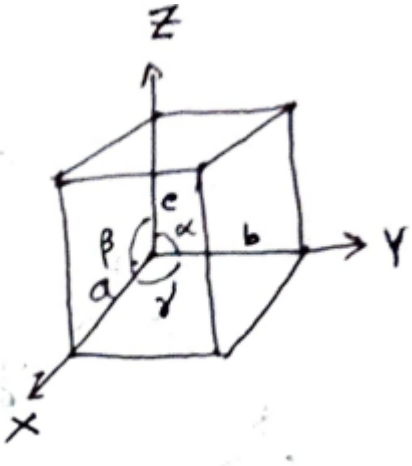
Crystalline Solid	Non-crystalline Solid / Amorphous
Have defined geometric shape	Does not have defined shape
Symmetry	No symmetry
Sharp melting point	Exponential melting point
Anisotropic (Direction dependent)	Isotropic (Direction independent)
Shows conductivity	Does not show conductivity
Table salt, diamond, mostly metals	Rubbers, glass

Unit Cell

Unit cell is the smallest repeating unit that forms the total symmetry of a crystal.

There are certain properties of an unit cell which are called the **Lattice Parameter**. The lattice parameters are :

1. Axial Length `( a , b , c )`
2. Axial Angle (α, β, γ)



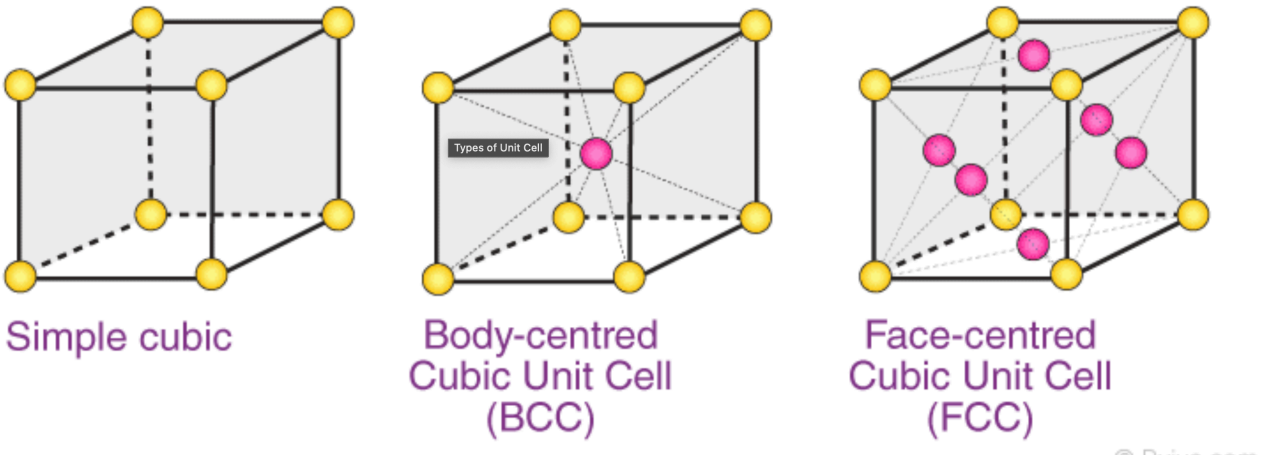
- Lattice parameter refers to the physical dimension of unit cell.

Different lattice parameters can form different kind of crystal unit or unit cell. Some are given below :

Crystal System	Lattice Parameter
Triclinic	$\alpha \neq \beta \neq \gamma \neq 90^\circ$ $a \neq b \neq c$
Monoclinic	$\alpha = \beta = 90^\circ \neq \gamma$ $a \neq b \neq c$
Orthohombic	$\alpha = \beta = \gamma = 90^\circ$ $a \neq b \neq c$
Cubic	$\alpha = \beta = \gamma = 90^\circ$ $a = b = c$
Tetragonal	$\alpha = \beta = \gamma = 90^\circ$ $a = b \neq c$
Hexagonal	$\alpha = \beta = 90^\circ, \gamma = 120^\circ$ $a = b \neq c$

Unit cell can be broadly divided into 2 categories.

- **Primitive / Simple :** Lattice points lie only at corners
  - Effective number of lattice point = 1.
- **Non-Primitive :** Lattice points lie at corners and other locations such as inside or surface.
  - Effective number of lattice point > 1.
  - This type of unit cell can be broadly classified as following categories :
    - **Body Centered :** Lattice point are every corner and at the center of the body.
    - **Face Centered :** Lattice point at every corner and at the center of the each 6 surfaces.
    - **Base Centered :** Lattice point at every corner and at the center of 2 parallel surface.



Number of Lattice Point and Packing Factor

$$N = \frac{N_c}{8} + N_i + \frac{N_f}{2}$$

Here,
N = Effective Lattice Point
N_c = Number of Lattice Point at corners
N_i = Number of Lattice Point inside
N_f = Number of Lattice Point at surface

Density of Crystal Matter

$$\rho = \frac{\text{mass per unit cell}}{\text{volume of unit cell}}$$

$$= \frac{\text{number of atom} \times \text{mass of one atom}}{V}$$

$$= \frac{n \times \frac{M}{N_A}}{V}$$

$$= \frac{nM}{N_A V}$$

Here,
n = Number of Lattice Point, not the number of atom actually.

Packing Factor

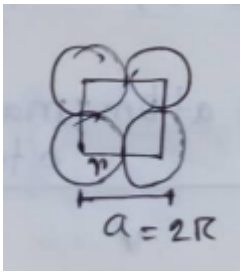
Packing factor is the fraction of space occupied by the constituent particles (atoms, ions, or molecules) in a unit cell of a crystal.

$$\text{Packing Factor} = \frac{\text{Volume of all atoms in unit cell}}{\text{Volute of unit cell}}$$

$$\therefore P.F. = \frac{N \times \frac{4}{3}\pi r^3}{a^3}$$

For a Simple Cube Unit Cell :

In a simple cubic structure, $a = 2r$
here,
a = Length of a side of the cubic structure
r = Radius of an atom



And the number of effective lattice is,

$$N = \frac{N_c}{8} + N_i + \frac{N_f}{2} = \frac{8}{8} + 0 + 0 = 1$$

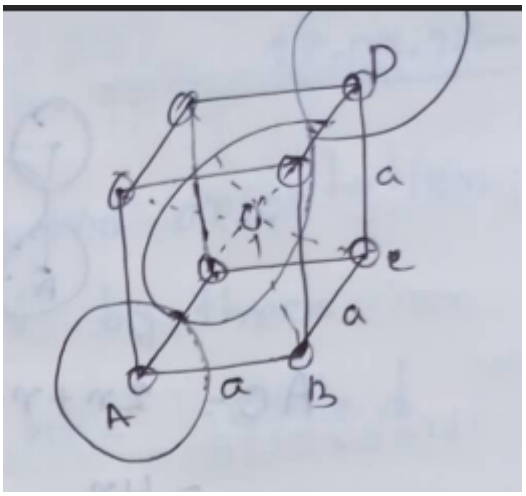
$$(P.F.)_{\text{Simple Cube}} = \frac{1 \times \frac{4}{3}\pi r^3}{(2r)^3}$$

$$= \frac{\frac{4}{3}\pi r^3}{8 \times r^3}$$

$$= \frac{\pi}{6} = 0.52 = 52\%$$

$$\text{Empty Space} = 100\% \text{ - } 52\% = 48\%$$

For a Body Centered Cubic Unit Cell



In this figure,

$$AD = r + 2r + r = 4r$$

Again,

$$AC^2 = AB^2 + BC^2$$

$$AD^2 = AC^2 + CD^2$$

$$\Rightarrow AD^2 = AB^2 + BC^2 + CD^2$$

$$\Rightarrow (4r)^2 = 3a^2$$

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

Number of effective lattice point would be,

$$N = \frac{N_c}{8} + N_i + \frac{N_f}{2} = \frac{8}{8} + 1 + 0 = 2$$

Now, the Packing Factor will be,

$$(P.F.)_{\text{BCC}} = \frac{N \times \frac{4}{3}\pi r^3}{a^3}$$

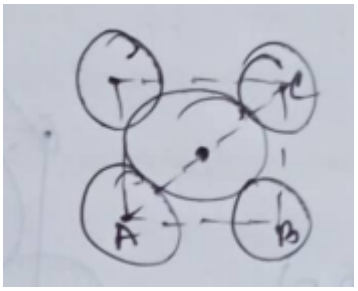
$$= \frac{2 \times \frac{4}{3}\pi(\frac{\sqrt{3}}{4}a)^3}{a^3} = 68\%$$

$$\text{Empty Space} = 32\%$$

Here, we can come to the conclusion that Body Centered Cubic Unit Cells are more closely packed than Simple Cubic Unit Cell.

$$\text{Higher packing factor} \rightarrow \text{more space occupied by atoms.}$$

For a Face Centered Cubic Unit Cell



Surface of an unit cell,

$$AC = r + 2r + r = 4r$$

Again,

$$AC^2 = AB^2 + BC^2 = 2a^2$$

$$\Rightarrow 4r = \sqrt{2}a$$

$$\therefore a = 2\sqrt{2}r$$

Number of effective lattice point,

$$N = \frac{N_c}{8} + N_i + \frac{N_f}{2} = \frac{8}{8} + 0 + \frac{6}{2} = 4$$

Now, the Packing Factor will be,

$$(P.F.)_{\text{FCC}} = \frac{4 \times \frac{4}{3}\pi r^3}{(2\sqrt{2}r)^3} = 74\%$$

$$\text{Empty Space} = 26\%$$

Here, Face Centered Cubic is the most closely pact structure among the structure we discussed so far.

Crystal Place

Crystal plane are some imaginary plane inside a crystal in which large concentration of atom are present.

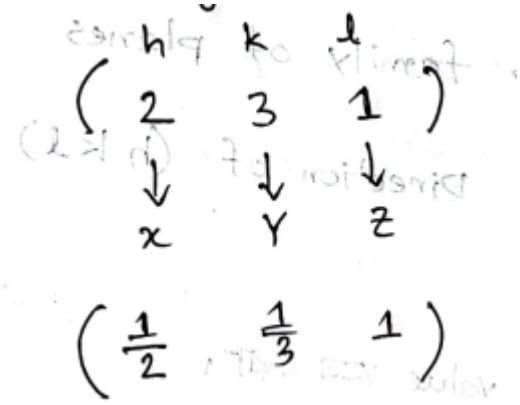
Miller Indices

The position and orientation of a crystal place is describe by there integers `h, k , l` are called Miller Indices.

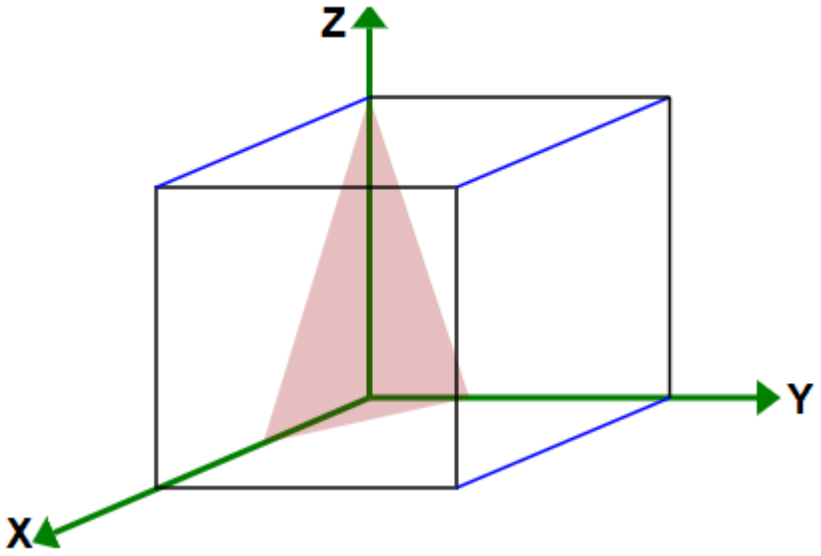
`( h k l )` ---> Refers to single plane
`{ h k l }` ---> Refers to family of planes
`[ h k l ]` ---> Refers to direction of `( h k l )` plane
`< h k l >` ---> Family of direction

Example of drawing of plane (2 3 1)

We first take reciprocal of (2 3 1)



Then we go half of the total length on X-axis, one third on the Y-axis and one full on the Z-axis. We create a plane by connecting those points as per the following diagram.



Exercise :

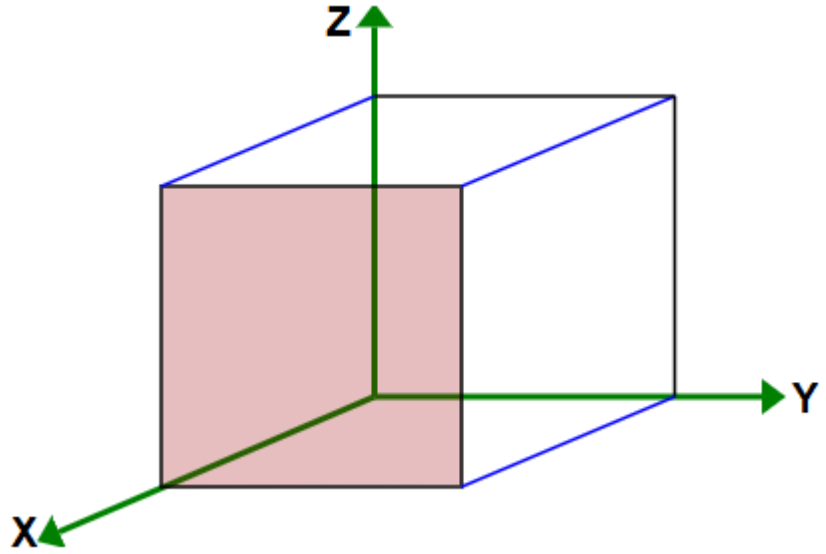
- `( 1 0 0 )`

(1 0 0)

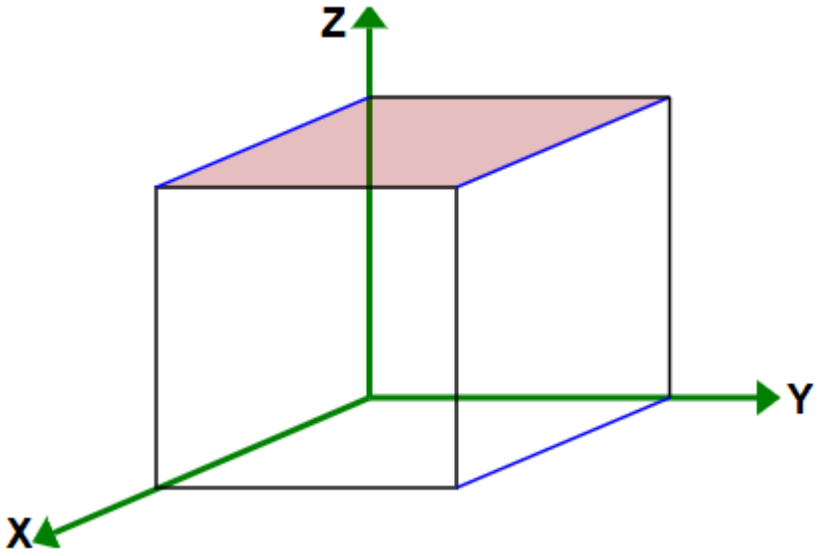
$\left(\frac{1}{1} \quad \frac{1}{0} \quad \frac{1}{0}\right)$

(1 ∞ ∞)

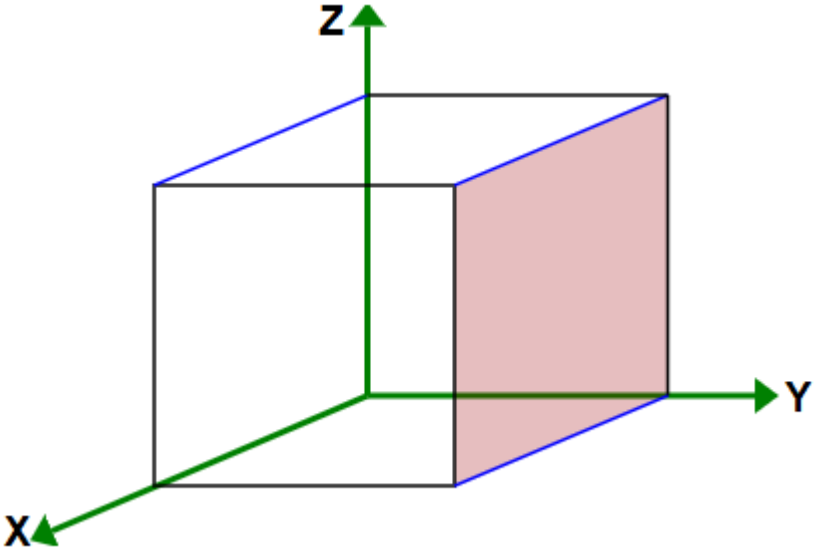
x y z



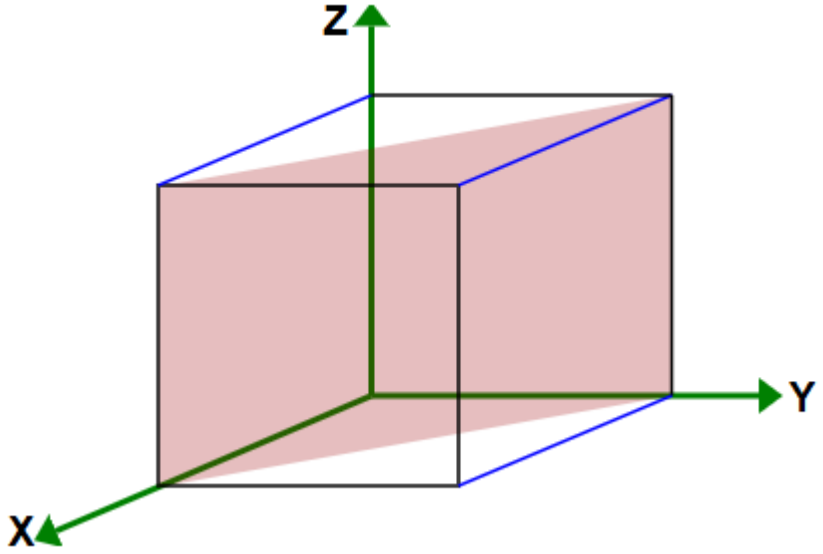
- `( 0 0 1 )`



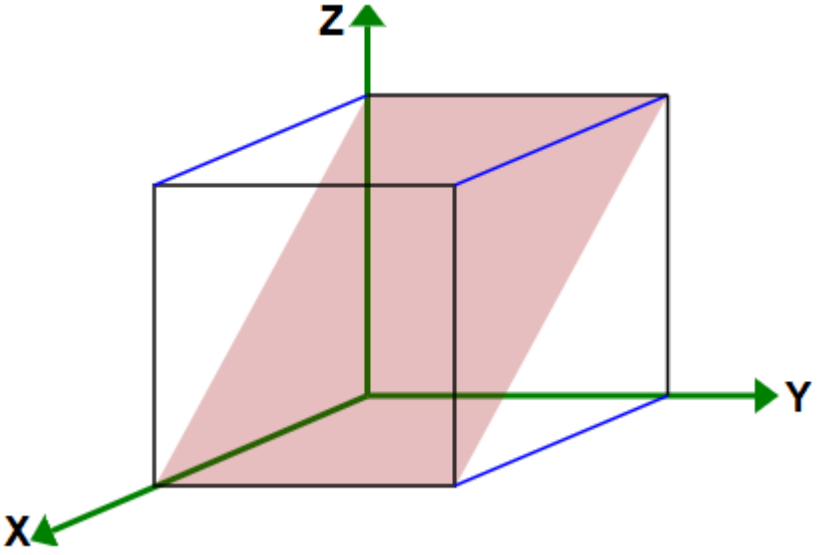
- `( 0 1 0 )`



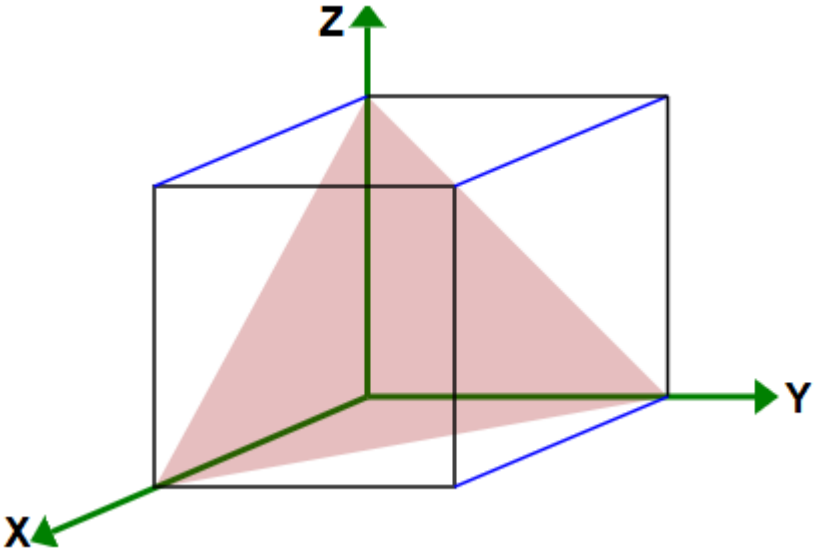
- `( 1 1 0 )`



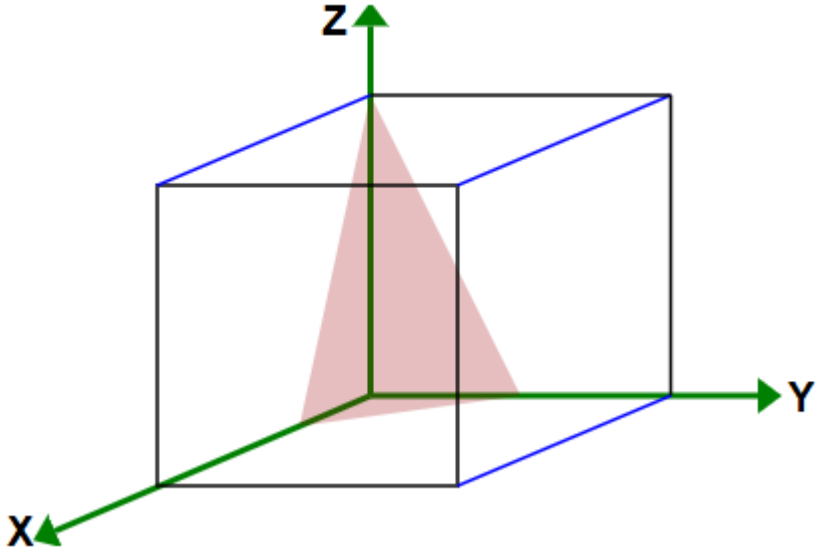
- `( 1 0 1 )`



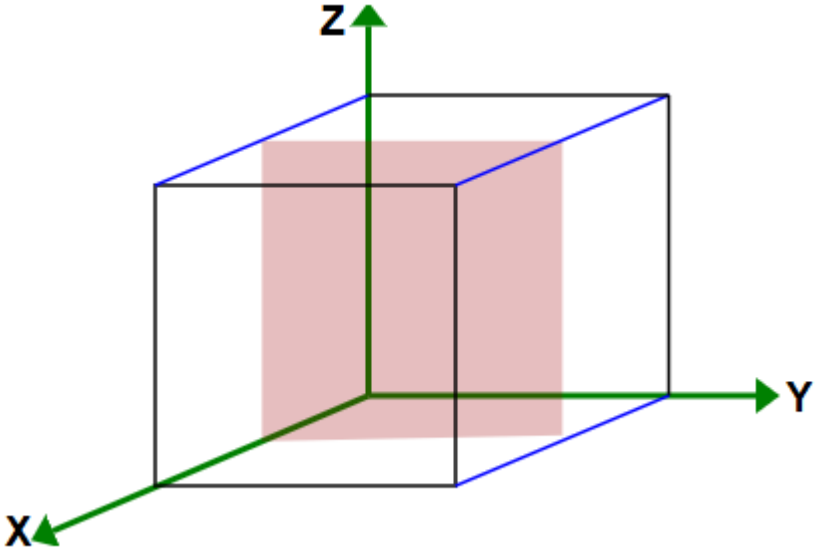
- `( 1 1 1 )`



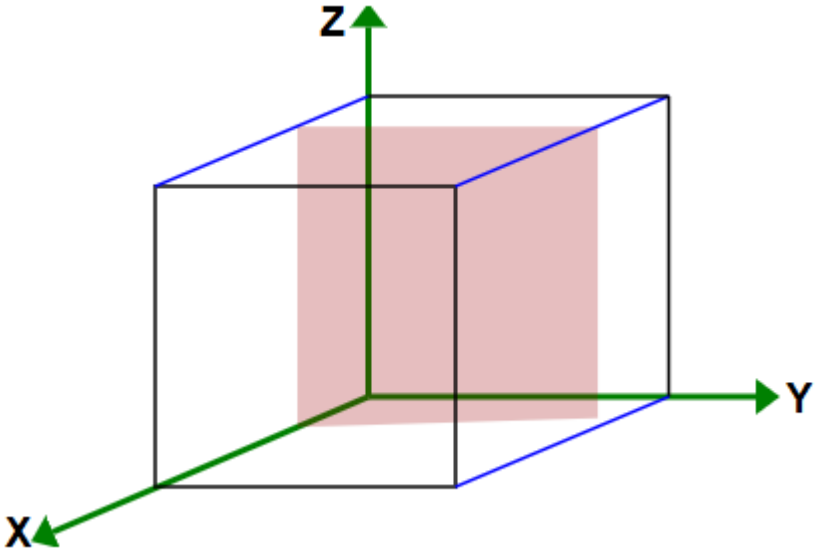
- `( 3 2 1 )`



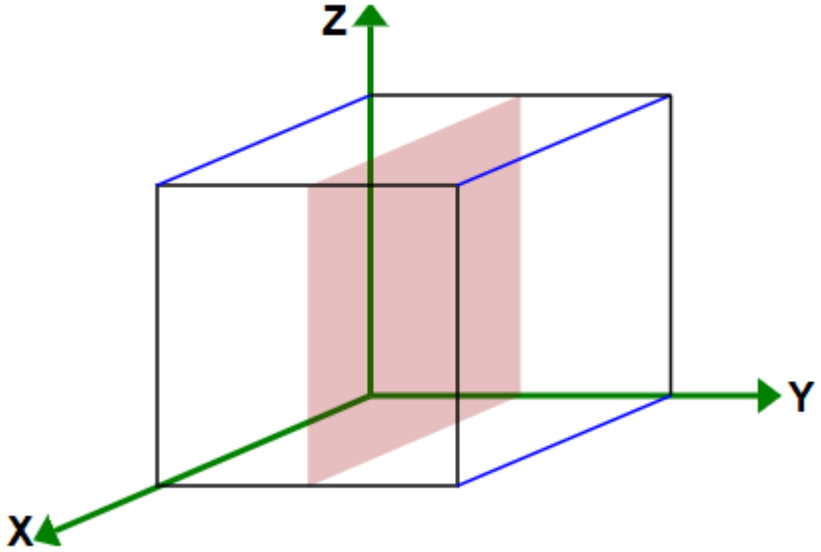
- `( 2 0 0 )`



- `( 3 0 0 )`

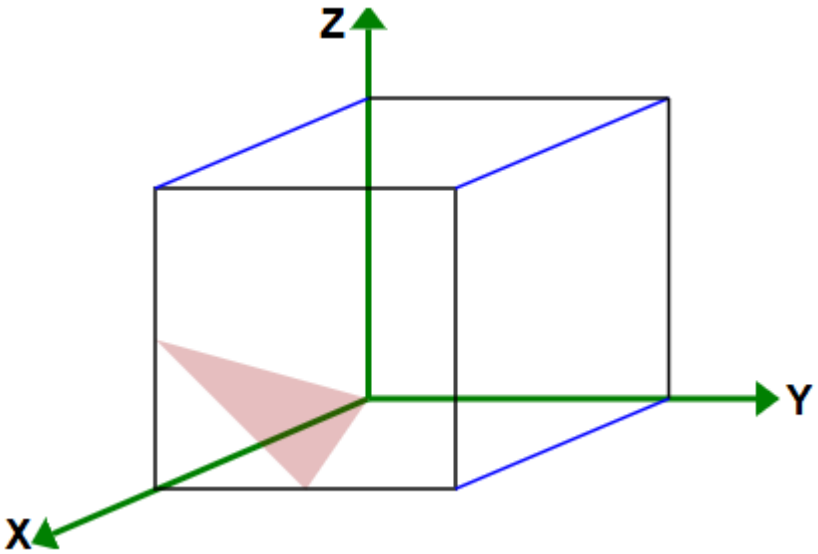


- `( 0 2 0 )`



Sometimes h, k or l can be represented as negative integer or given a bar $(\bar{1})$ like this above them, which generally indicates change in origin. In general the origin is at `( 0 0 0 )` but if we use negative integer on X-axis the origin become `( x 0 0 )` where x is the length of the plane along with x-axis. For example:

- $(\bar{1}\,2\,2)$



Here the origin is on the lower left point. Similarly negative indices can be applied to y-axis and z-axis.

Direction of Miller's plane

To find the direction of Miller's plane we first need to consider the origin of the lattice point (considering negative indices as well). After that we need to divide every index by $max(h, k, l)$.

We need to find the specific point after that and draw a line from the origin and we will have our intended direction. For example

$[2\ 1\ 0]$ will be transformed to $\frac{2}{2},\ \frac{1}{2},\ \frac{0}{2}$ as 2 is the maximum between $h,\ k$ and l. then we will draw a line from the origin as per the following diagram.