ATOMIC AND CRYSTAL STRUCTURE OF MATERIALS

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Continued from last time

Atomic Arrangement in crystals

The seven systems used are summarised as follows:

1. Cubic $a = b = c; \quad \alpha = \beta = \gamma = 90^o$
2. Tetragonal $a = b \neq c; \quad \alpha = \beta = \gamma = 90^o$
3. Orthorhombic $a \neq b \neq c; \quad \alpha = \beta = \gamma = 90^o$
4. Rhombohedral $a = b = c; \quad \alpha = \beta = \gamma \neq 90^o$
5. Hexagonal $a = b \neq c; \quad \alpha = \beta = 90^o, \gamma = 120^o$
6. Monoclinic $a \neq b \neq c; \quad \alpha = \beta = 90^o \neq \gamma$
7. Triclinic $a \neq b \neq c; \quad \alpha \neq \beta \neq \gamma \neq 90^o$

Atomic Arrangement in crystals

Some Materials the Crystallise in these Crystal Systems:

Crystal system	Example
Triclinic	$K_2S_2O_8, K_2Cr_2O_7$
Monoclinic	As_4S_4, KNO_2, $CaSO_4.2H_2O$, β-S
Rhombohedral	Hg, Sb, As, Bi, $CaCO_3$
Hexagonal	Zn, Co, Cd, Mg, Zr, NiAs
Orthorhombic	Ga, Fe_3C, α-S
Tetragonal	In, TiO_2, β-Sn
Cubic	Au, Si, Al, Cu, Ag, Fe, NaCl

Atomic Arrangement in crystals

Unit cell = building block for every crystal.

Within each system, there is one or more types of space lattice structures distinguished by differing degrees of symmetry within the unit cell.

E.g.

Cubic system $\Rightarrow$ 3 space lattices, viz: simple cubic, fcc & bcc

Hexagonal system $\Rightarrow$ only two lattices, the simple hexagonal and hexagonal close packed (hcp or cph).

Atomic Arrangement in crystals

- Physical properties depend more on shape and atomic arrangement of the unit cell than upon which atoms are present.

- Many properties also vary with crystallographic direction. Hence, the need to also specify various planes of atoms and directions within the crystal $\Rightarrow$ hence *Miller index notation*.

Atomic Arrangement in crystals

Indices of Planes

Plane – surface defined by length of its intercepts on the three crystal axes (the three edges of a unit cell).

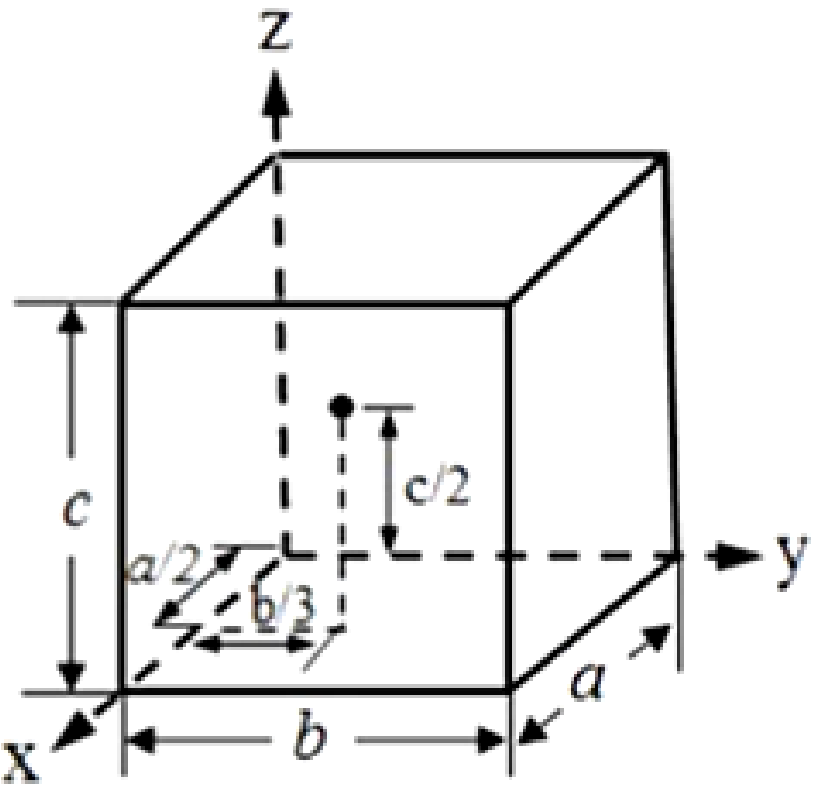
Intercepts are expressed in terms of the dimensions of unit cell, i.e. unit cell distances along the three axes.

Reciprocals of these intercepts reduced to the smallest three integers = ***Miller indices***.

Atomic Arrangement in crystals

Indices of Planes

- Position of any point in a unit cell is given by its coordinates or distances from the x, y and z axes in terms of the lattice vectors a, b and c.



- Thus the point located at a/2 along x axis, b/3 along y axis and c/2 along z axis, as shown in the figure below, has the coordinates: $\frac{1}{2}, \frac{1}{3}, \frac{1}{2}$.

Atomic Arrangement in crystals

Indices of Planes

- Planes in a crystal are described by notations called **Miller indices**.
- Miller indices of a plane, indicated by h k l, are given by the reciprocal of the intercepts of the plane on the three axes.
- The plane, which intersects X-axis at 1 (one lattice parameter) and is parallel to Y and Z axes, has Miller indices $h = 1/1 = 1$, $k = 1/\infty = 0$, $l = 1/\infty = 0$. It is written as (hkl) = (100).
- Miller indices of some other planes in the cubic system are shown in the figures in the next slide

Atomic Arrangement in crystals

For a plane with intercepts 1, 1, 1:

- Reciprocals = 1, 1, 1
- Miller indices = (111).

For a plane with intercepts 2, ∞, 1 (i.e. parallel to *OY* axis)

- Reciprocals = ½, 0, 1
- Miller indices = (102) when reduced to lowest integer values.

Atomic Arrangement in crystals

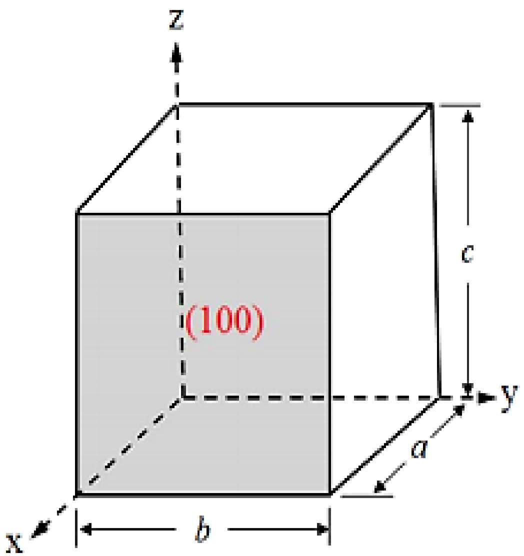
Planes can also have negative intercept e.g.:

- If a plane has –ve intercept, the index will be –ve, written with a bar above the number, $(1\bar{1}0)$.

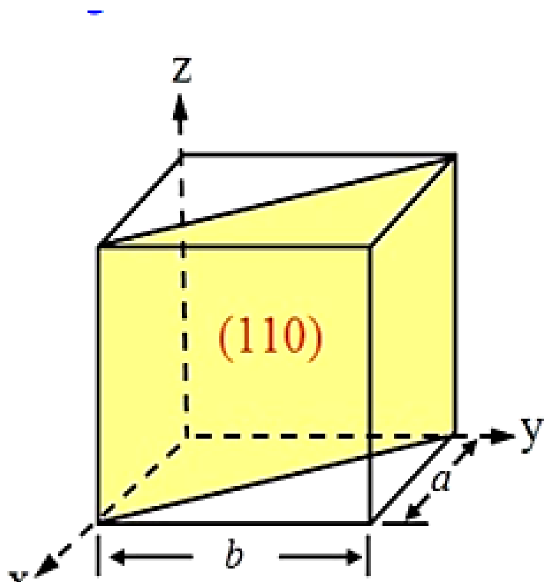
- And for intercepts 1, 1,-1/2; h k l = 1 1 -2. This is denoted as $(11\bar{2})$

Atomic Arrangement in crystals

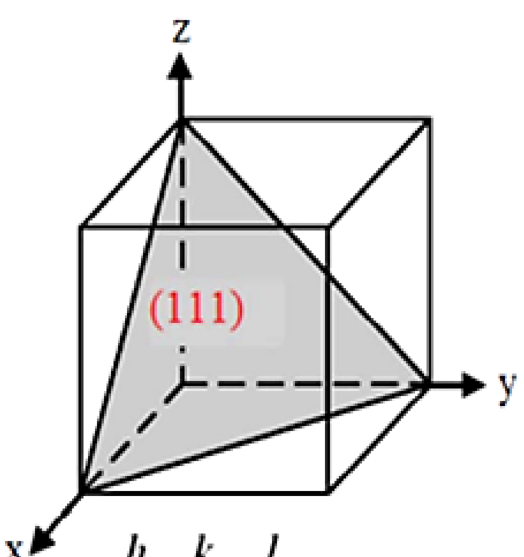
- Miller indices of some other planes in the cubic system are shown in the figures in the next slide



$$\begin{matrix} h & k & l \\ \frac{1}{1} & \frac{1}{\infty} & \frac{1}{\infty} \end{matrix} = (100)$$



$$\begin{matrix} h & k & l \\ \frac{1}{1} & \frac{1}{1} & \frac{1}{\infty} \end{matrix} = (110)$$



$$\begin{matrix} h & k & l \\ \frac{1}{1} & \frac{1}{1} & \frac{1}{1} \end{matrix} = (111)$$

Atomic Arrangement in crystals

Family of planes {hkl}

Paranthesis (hkl) around a set of indices signify a single set of parallel planes.

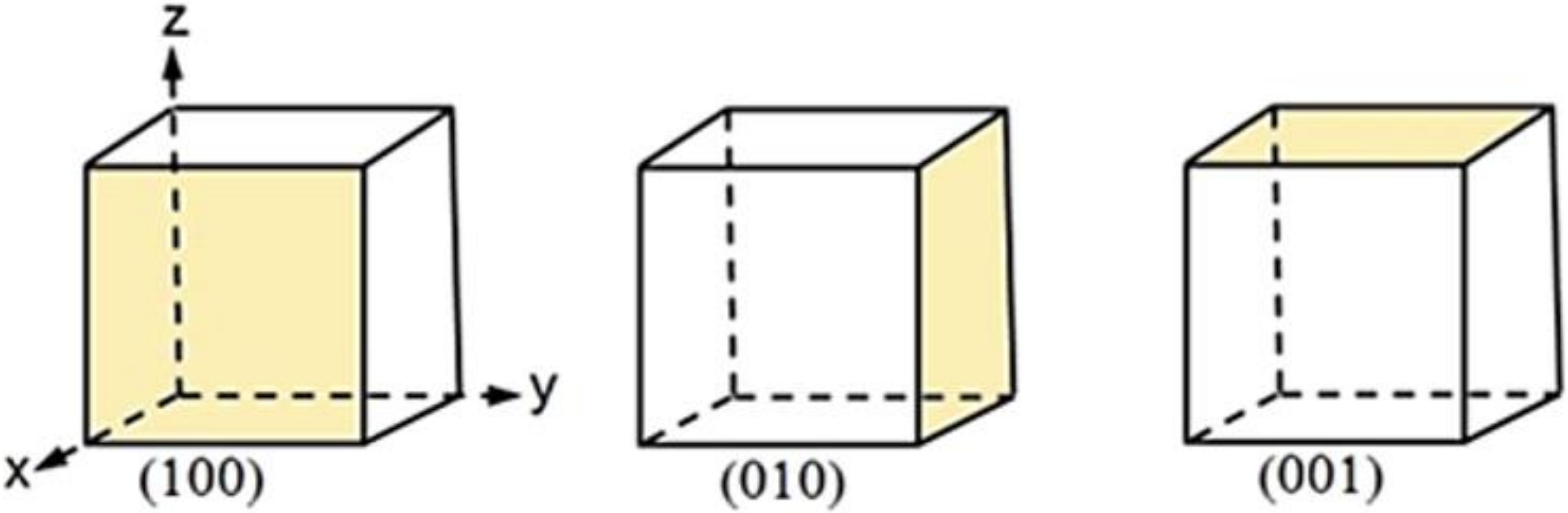
Curly brackets or braces {hkl} signify planes of a form, i.e., a family or a set of equivalent planes.

Thus for the cubic crystal, {110} invludes six sets of planes: (110), (101), (011), $(1\bar{1}0)$, $(10\bar{1})$ and $(01\bar{1})$.

Reversal of the signs of all indices merely denotes another parallel plane. Thus $(\bar{1}\bar{1}0)$ is parallel to (110) and (101) to $(10\bar{1})$.

Atomic Arrangement in crystals

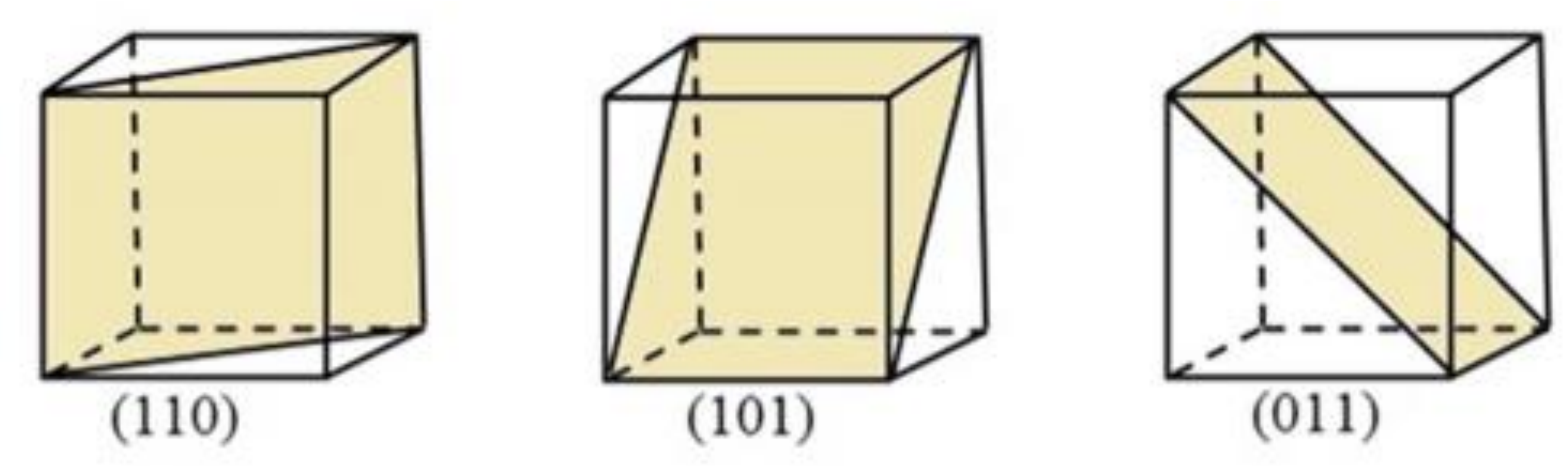
Family of planes {hkl}



{100} Family of planes

Atomic Arrangement in crystals

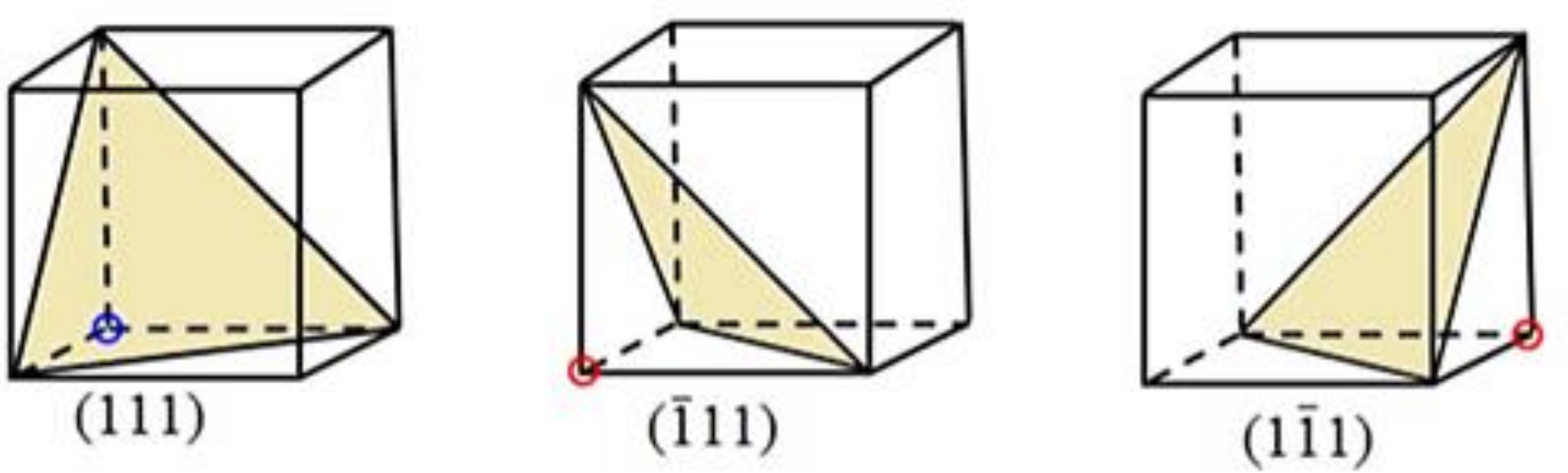
Family of planes {hkl}



{110} Family of planes

Atomic Arrangement in crystals

Family of planes {hkl}



{111} Family of planes

Note the apparent shift of the origin from blue to red circle for the negative indices

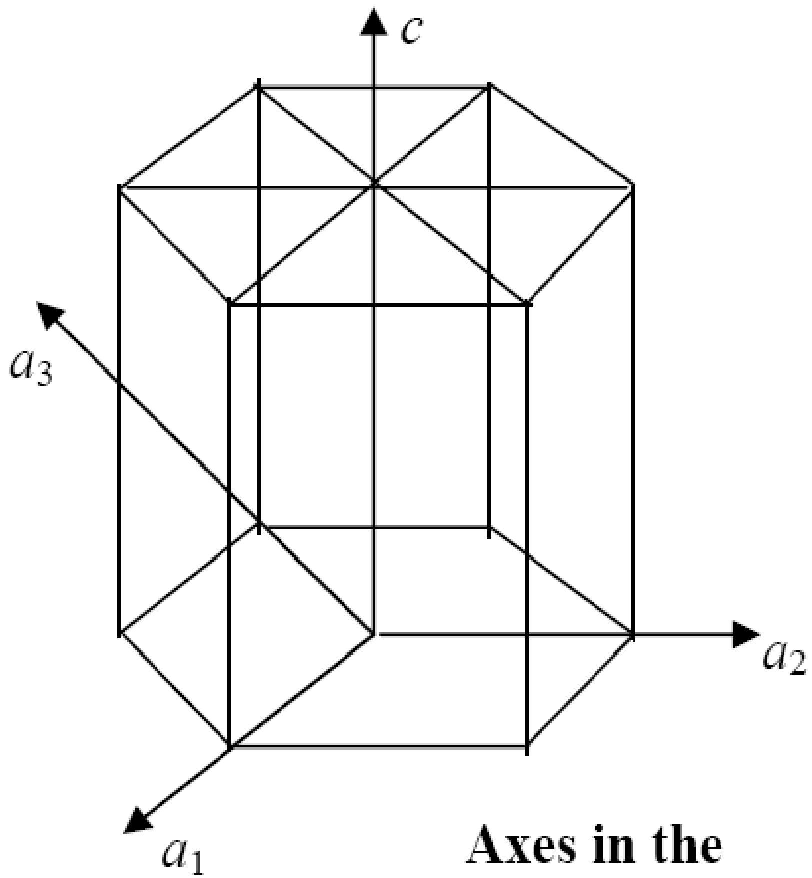
Atomic Arrangement in crystals

Planes in Hexagonal system

For hexagonal system, alternative indexing is used.

Four numbers *h, k, i, l* are used in the ***Miller-Bravais*** - the intercepts on four axes, a_1, a_2, a_3, and c as shown in the figure.

Treatment same as *Miller indices*.

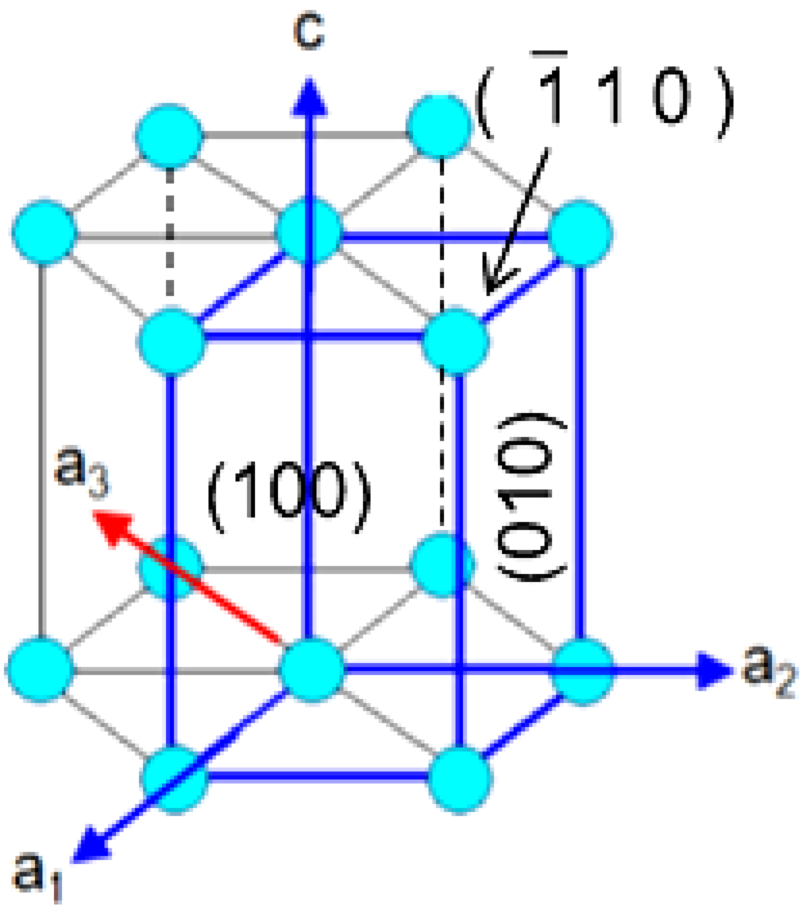


Axes in the hexagonal lattice

Atomic Arrangement in crystals

Planes in Hexagonal system

- In the cubic system all the faces of the cube are equivalent, that is, they have similar indices.
- However, this is not the case in the hexagonal system. The six prism faces for example have indices (100), (010), ($\bar{1}$10), ($\bar{1}$00), (0$\bar{1}$0), (1$\bar{1}$0), which are not same.



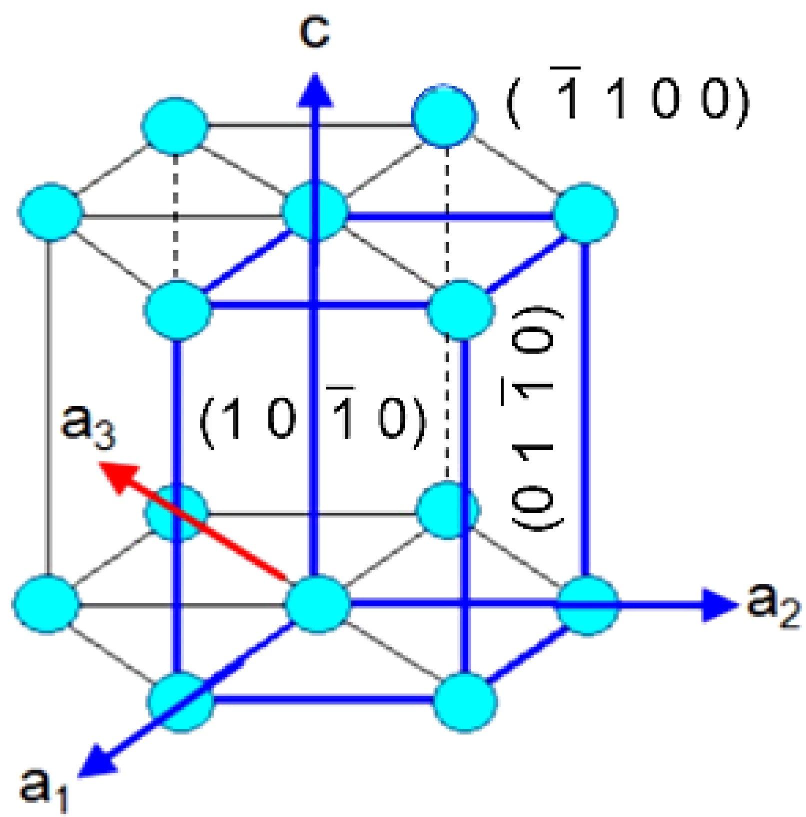
Atomic Arrangement in crystals

Planes in Hexagonal system

- In order to address this, a fourth axis (a_3) which is opposite to the vector sum of a1 and a_2 is used and a corresponding fourth index is used along with hkl.
- Therefore the indices of a plane is given by (*hkil*), where $i = -(h+k)$. Sometime *i* is replaced with a dot and written as (*h k . l*)

Atomic Arrangement in crystals

The indices of six faces now become $(10\bar{1}0)$, $(01\bar{1}0)$, $(\bar{1}100)$, $(\bar{1}010)$, $(0\bar{1}10)$, $(1\bar{1}00)$ which are now equivalent and belong to the $\{10\bar{1}0\}$ family of planes.

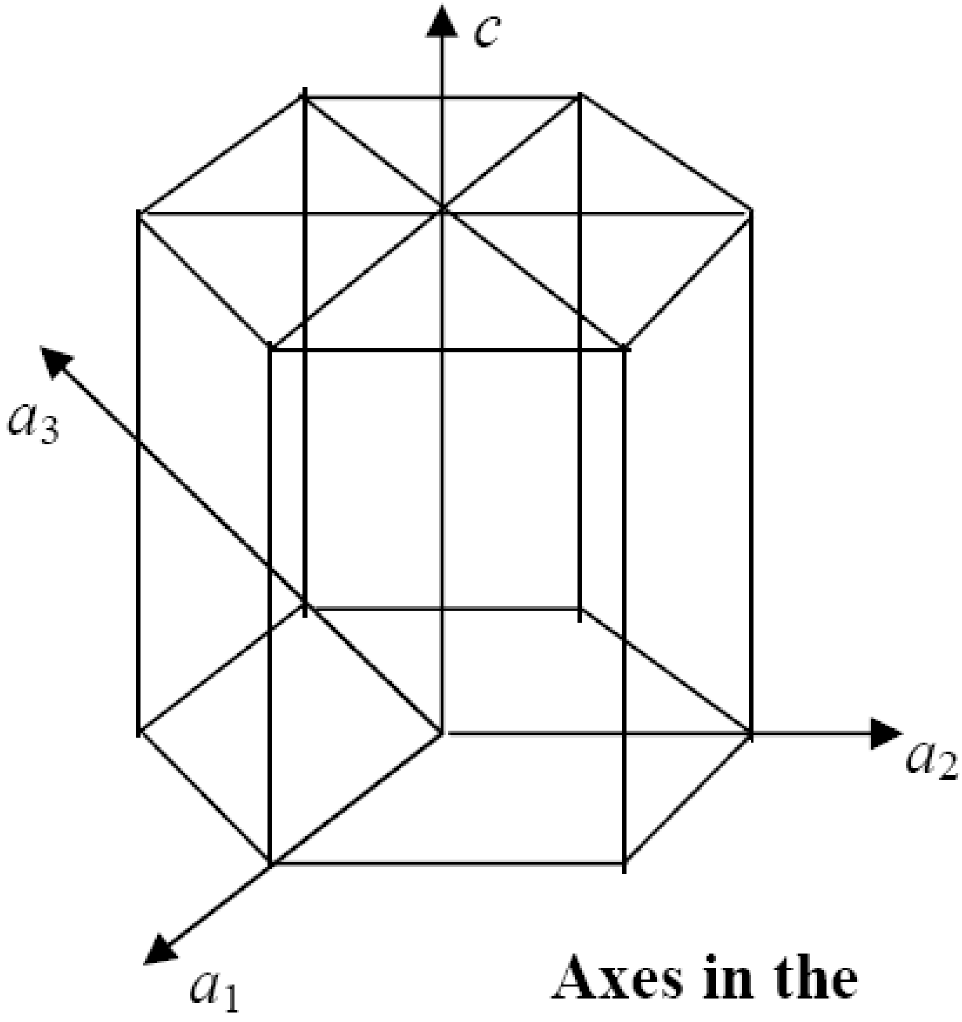


Atomic Arrangement in crystals

Note:

The first three indices are not independent but must satisfy:

$$h + k + i = 0$$



Axes in the hexagonal lattice

Atomic Arrangement in crystals

Interplanar Spacing

The spacing between planes in a crystal is known as interplanar spacing and is denoted as dhkl

In the cubic system spacing between the (hkl) planes is given as $\frac{1}{d^2} = \frac{1}{a^2}(h^2 + k^2 + l^2)$

For example, d_{hkl} of {111} planes $d_{111} = a\sqrt{3}$

and

In the Tetragonal system $\frac{1}{d_{hkl}^2} = \frac{1}{a^2}(h^2 + k^2) + \frac{1}{c^2} l^2$

Atomic Arrangement in crystals

Interplanar Spacing

In Hexagonal system $$\frac{1}{d_{hkl}^2} = \frac{1}{a^2}h^2 + \frac{1}{a^2}k^2 + \frac{1}{c^2}l^2$$

In Orthorhombic system

$$\frac{1}{d_{hkl}^2} = \frac{4}{3a^2}(h^2 + hk + k^2) + \frac{1}{c^2}l^2$$

or $$\frac{1}{d_{hkl}^2} = \frac{1}{a^2}h^2 + \frac{1}{b^2}k^2 + \frac{1}{c^2}l^2$$

Atomic Arrangement in crystals

Indices of Crystal Directions

Direction = defined as successive motion parallel to each of the three axes necessary to move from the origin to another point, which lies in the required direction.

Atomic Arrangement in crystals

Directions in the Cubic System

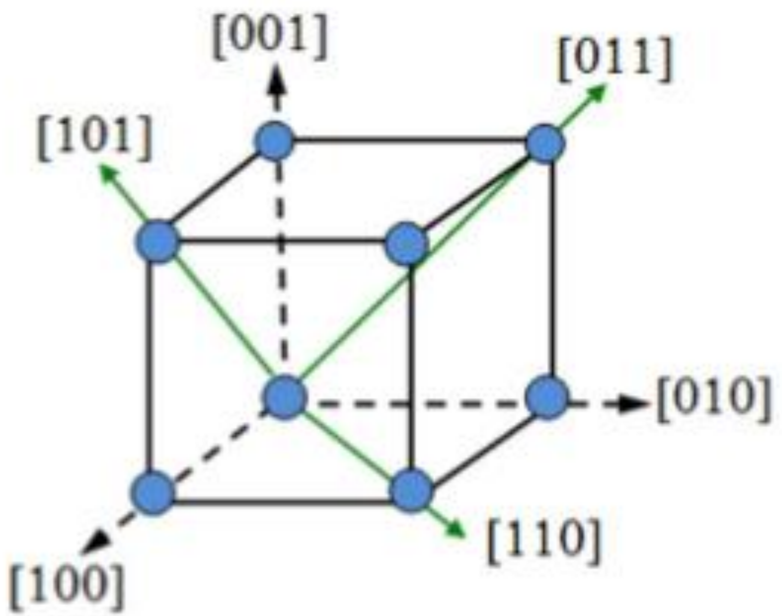
- The directions in a crystal are given by specifying the coordinates (u, v, w) of a point on a vector (r_{uvw}) passing through the origin, $r_{uvw} = ua + vb + wc$. It is indicated as [uvw].

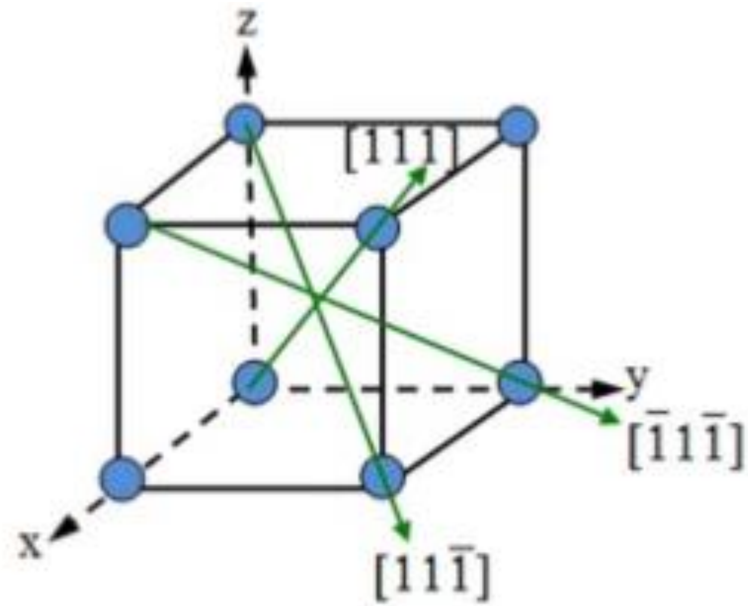
- For example, the direction [110] lies on a vector r_{110} whose projection lengths on x and y axes are one unit (in terms of unit vectors ***a*** and ***b***).

- Directions of a form or family like [110], [101], [011] are written as <110> (using caret < >).

- Reciprocals are not used in indices of direction.

Atomic Arrangement in crystals





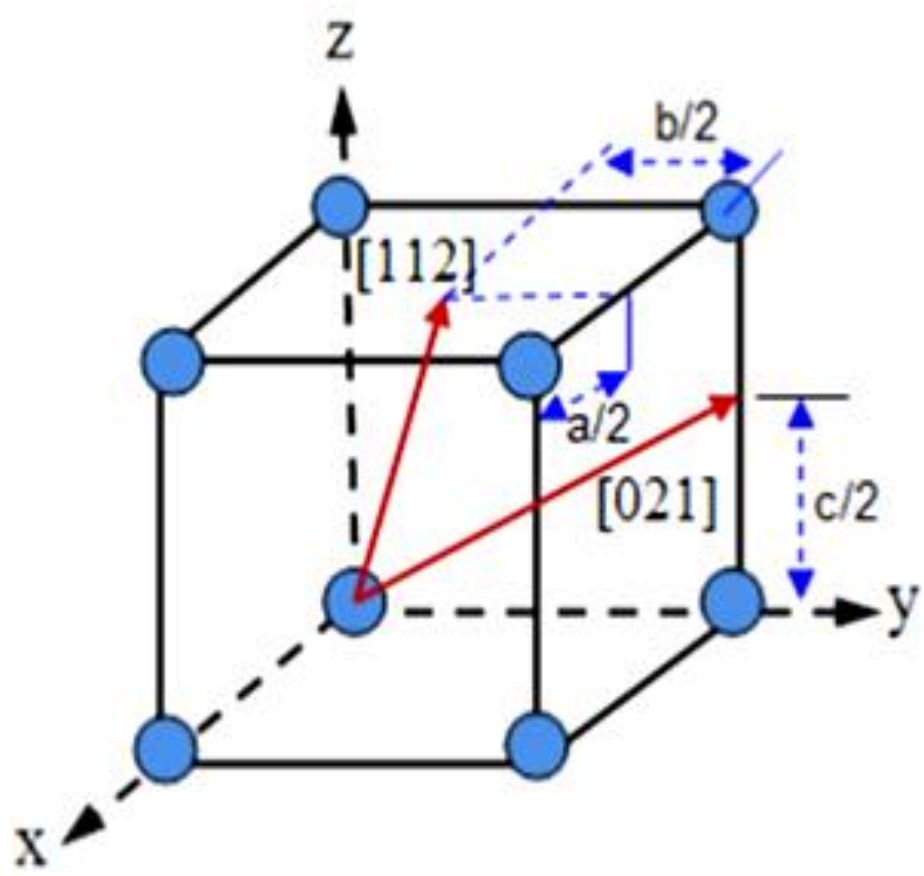
<110> = Family of directions of face diagonals

<111> = Family of directions of major diagonals

<100> = Family of directions along the axes

Atomic Arrangement in crystals

- The line which passes through uvw will also pass through $2u2v2w$ and $\frac{1}{2}u\ \frac{1}{2}v\ \frac{1}{2}w$.
- Hence [uvw], [2u2v2w] and [½u ½v ½w] are same and written as [uvw].
- Fractions are converted in to integers (as shown in the figure below) and reduced to lowest terms.



Atomic Arrangement in crystals

- To determine a direction of a line in the crystal:
- Find the coordinates of the two ends of the line and subtract the coordinates (Head to Tail) OR draw a line from the origin parallel to the line and find its projection lengths on x, y and z axis in terms of the unit vectors a, band c.
- Convert fractions, if any, in to integers and reduce to lowest term.
- Enclose in square brackets [uvw]

Atomic Arrangement in crystals

Directions in the Hexagonal System

- Like planes, directions in the hexagonal system are also written in terms of four indices as [uvtw].
- If [UVW] are indices in three axes then it can be converted to four-axis indices [uvtw] using the following relations.

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

$u = (2U - V)/3; \quad v = (2V - U)/3; \quad t = -(u + v) = -(U + V)/3$

$w = W$

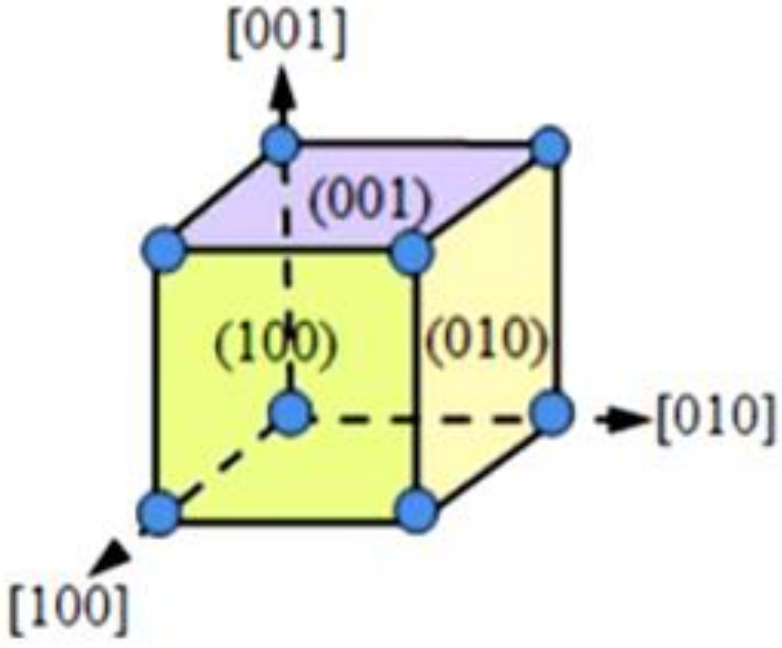
Ex: $[100] = [2\bar{1}\bar{1}0]$, $[210] = [10\bar{1}0]$

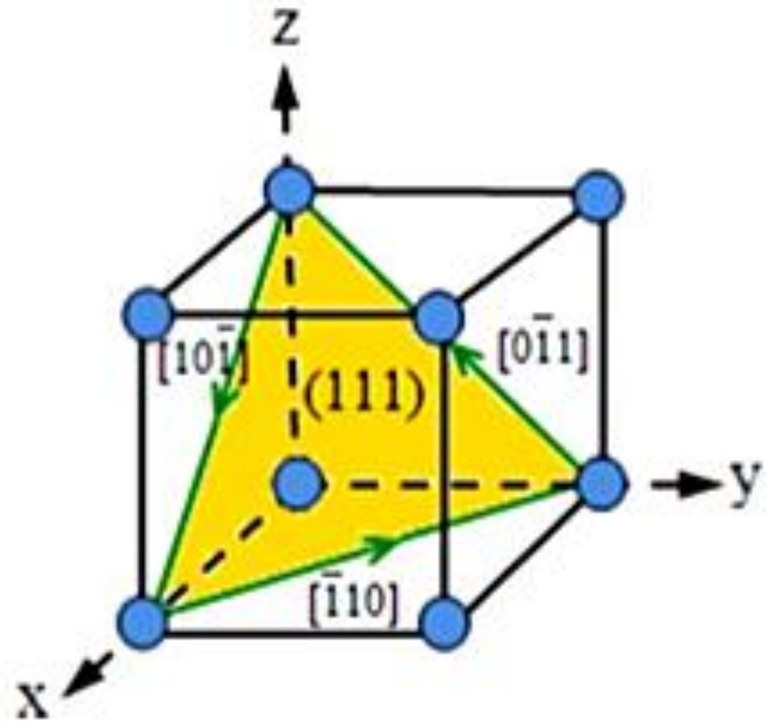
Atomic Arrangement in crystals

Relationship between direction and planes

- In the cubic system planes and directions having same indices are perpendicular to each other i.e. if [uvw] direction is perpendicular to (hkl) plane
- Then h = u, k = v and l = w. Ex: {100} planes and <100> directions are perpendicular to each other.
- If [uvw] direction is parallel to (hkl), that is if [uvw] lies in the plane (hkl) then hu+ kv+ lw= 0.
- For example, [$\bar{1}$ 1 0] lies in the plane (111), since 1.(-1) + 1.1 + 1.0 = 0

Atomic Arrangement in crystals





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