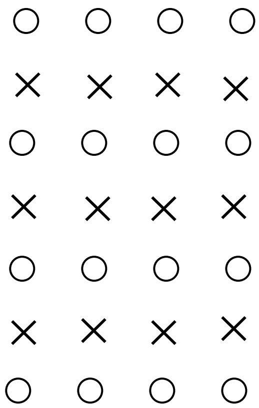
II crystal structure

2-1 basic concept

> Crystal structure = lattice structure + basis

> Lattice point: positions (points) in the structure which are identical.



> Lattice translation vector

> Lattice plane

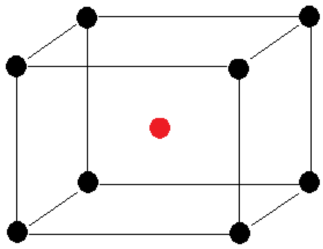
> Unit cell

> Primitive unit cell 【1 lattice point/unit cell】

- Several crystal structures:

  CsCl

  crystal structure = simple cubic (s.c.) lattice structure + basis



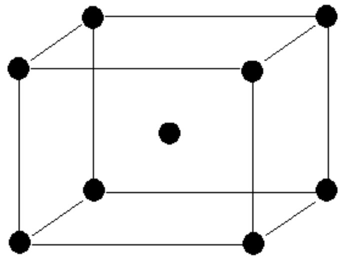
s.c. lattice structure is primitive

2 ions at each lattice point → basis= Cs^+  + Cl^- 

Fe (ferrite), Cr, Mo, W body-centered cubic (bcc)

bcc crystal structure =bcc lattice structure + basis

basis= 1 atom/lattice point

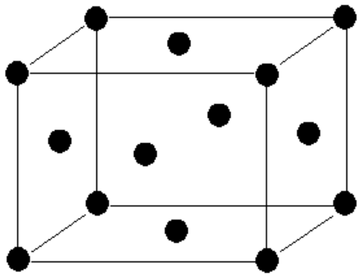


2 lattice points /bcc $\Rightarrow$ b.c.c is not primitive

Al, Au, Ag, Pt face-centered cubic (fcc)

fcc crystal structure =fcc lattice structure + basis

basis= 1 atom/lattice point

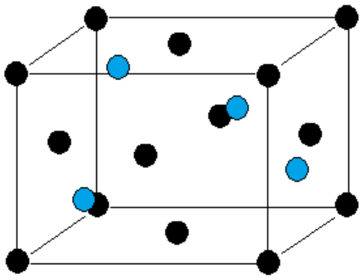


4 lattice points /fcc $\Rightarrow$ f.c.c is not primitive

GaAs, AlP, InP, ZnS, CdTe, HgTe

Zinc blende crystal structure = Ga (fcc) + As (fcc) (for GaAs)

fcc lattice structure

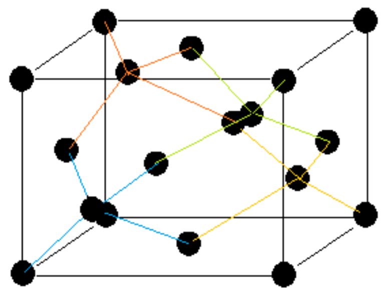


fcc lattice structure + basis

basis = Ga^{2+} ● + As^{2-} ● (for GaAs)

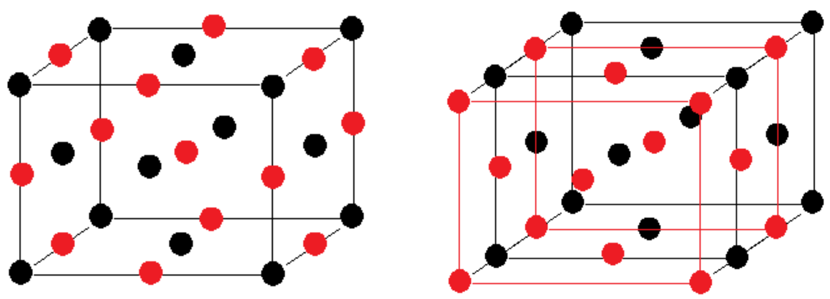
Si, Ge, diamond

diamond crystal structure = fcc lattice structure + basis



basis = 2 atoms/lattice point

NaCl = Na (fcc) + Cl (fcc)

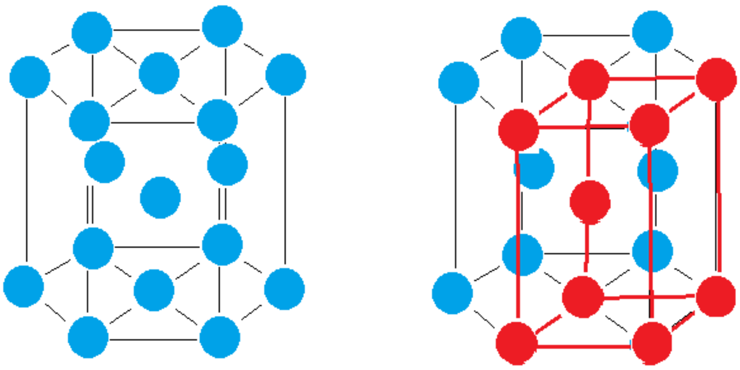


NaCl crystal structure = fcc lattice structure + basis

basis = Na^+ + Cl^-

Mg, Zn, hexagonal close packed (hcp)

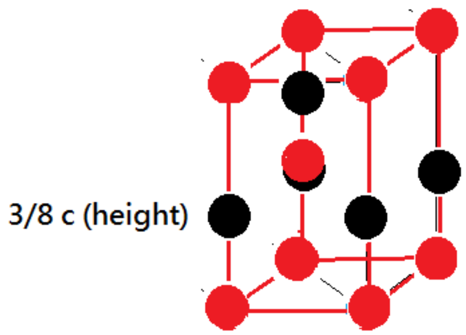
hcp crystal structure = simple hexagonal lattice + basis



basis = 2 atoms/lattice point

CdS, ZnO, ZnS

Wurtzite structure => Cd^{2+} hcp + S^{2-} hcp (for CdS)

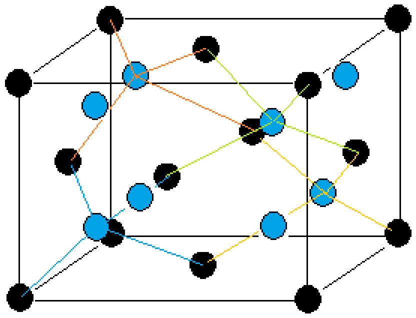


wurtzite structure = simple hexagonal lattice + basis

basis = 2 Cd^{2+} + 2 S^{2-} (for CdS)

CaF_2 Fluorite crystal structure

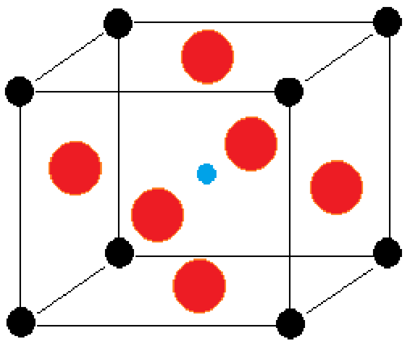
fluorite crystal structure = fcc lattice structure + basis



basis = Ca^{2+} + 2 F^- (at tetrahedral sites)

$BaTiO_3$, $CaTiO_3$ Perovskite crystal structure

perovskite crystal structure = simple cubic lattice structure + basis



basis =1 Ba^{2+} + 1 Ti^{4+} + 3 O^{2-}

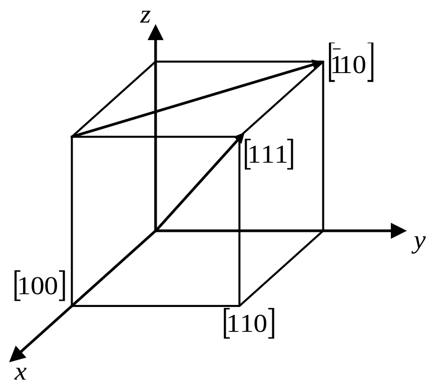
2-2 Miller Indices in a crystal

2-2-1 direction

The direction [u v w] is expressed as a vector

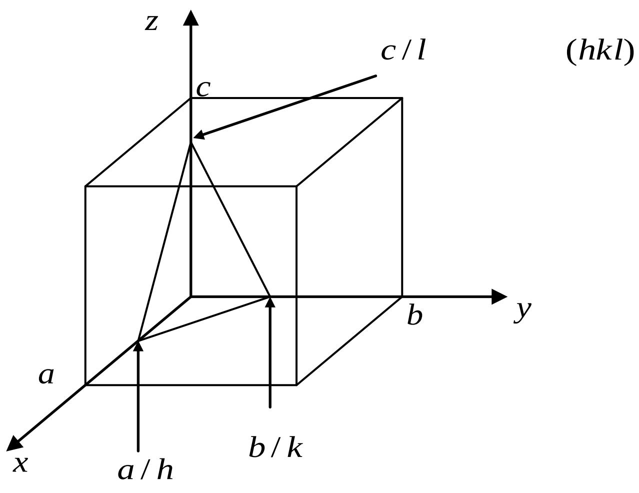
$$\vec{r} = u\hat{a} + v\hat{b} + w\hat{c}$$

The direction <u v w>are all the [u v w] types of direction, which are crystallographic equivalent.



2-2-2 plane

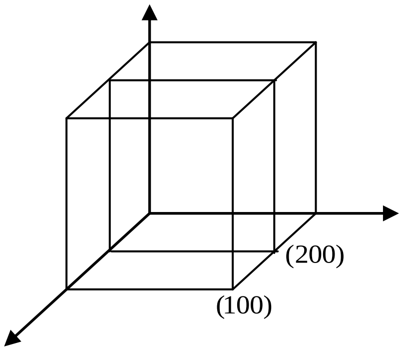
The plane (h k l) is is the Miller index of the plane.



$$\frac{x}{a/h} + \frac{y}{b/k} + \frac{z}{c/l} = 1$$

{h k l} are the (h k l) types of planes which are crystllographic equivalent.

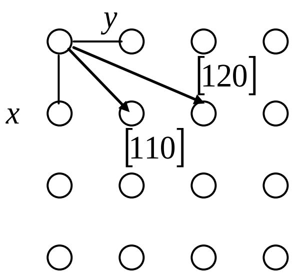
2-2-3 meaning of miller indices

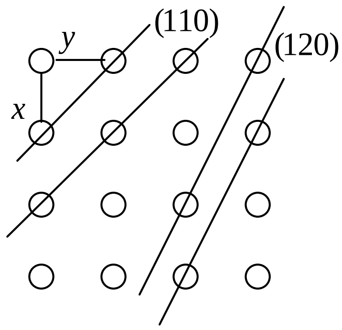


$$d_{200} = \frac{1}{2} d_{100}$$

>Low index planes are widely spaced.

>Low index directions correspond to short lattice translation vectors.



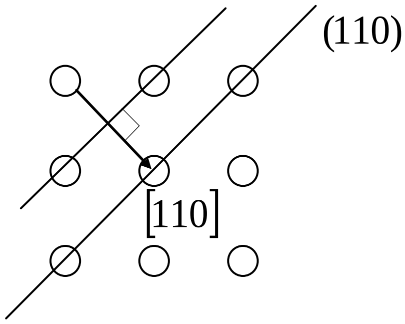


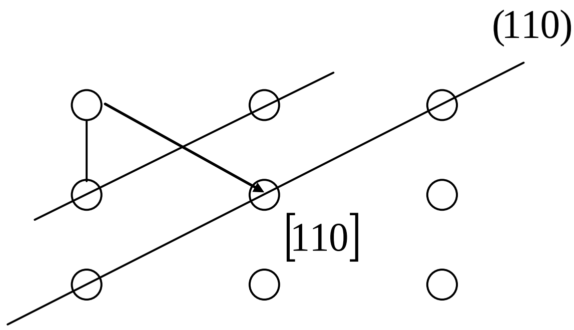
>Low index directions and planes are important for slip, and cross slip electron mobility.

2-3 Miller-Bravais indices

2-3-1 in cubic system

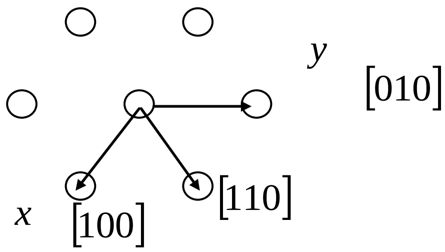
(1) Direction [h k l] is pepredicular to (h k l) plane in the cubic system, but not true for other crystal systems.





2-3-2 In hexagonal system

using Miller - Bravais indexing system：(hkil) and [hkil]



Reason (i)

Type [110] does not equal to [010] , but these directions are crystallographic equivalent.

Reason (ii)

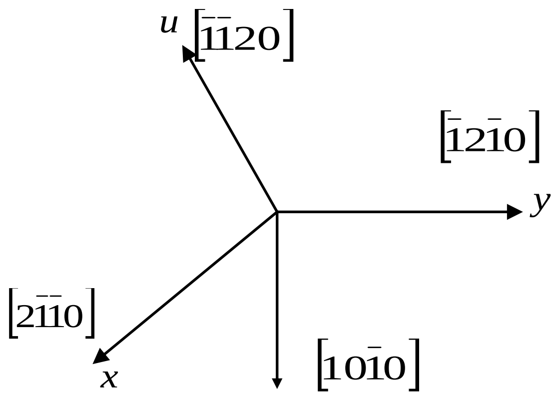
z axis is [001], crystallographically distinct from [100] and [010].

2-3-3 Miller-Bravais indices for the hexagonal system

(a) direction

The direction [h k i l] is expressed as a vector

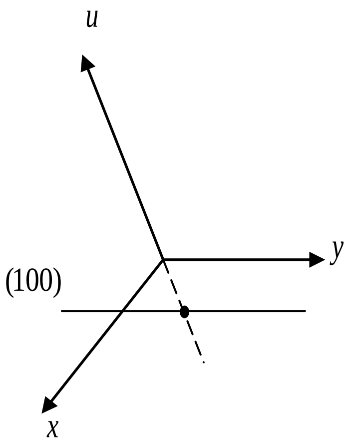
$$\vec{r} = h\hat{x} + k\hat{y} + i\hat{u} + l\hat{z}$$



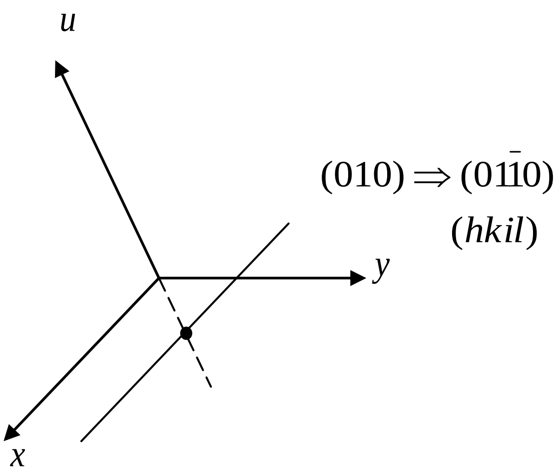
Note : $\frac{a}{3}[2\bar{1}\bar{1}0]$ is the shortest translation vector on the basal plane.

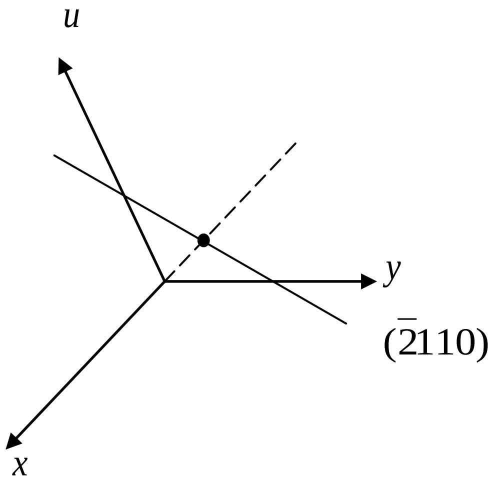
(b) planes (h k i l) ; h + k + i = 0

Plane (hkl) → (hkil)

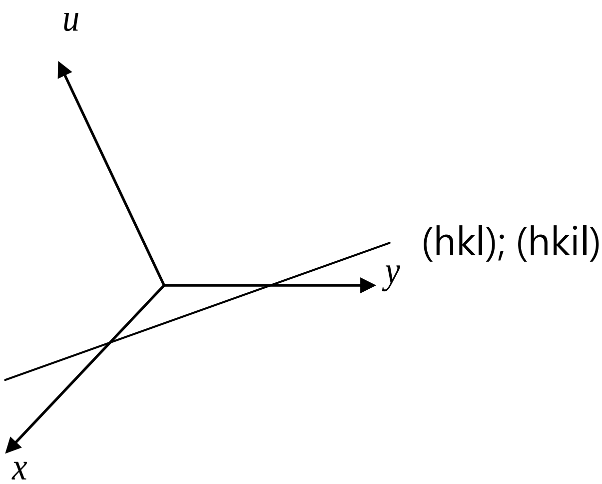


$$\underset{(hkil)}{(100) \Rightarrow (10\bar{1}0)}$$





Proof:



For plane (hkl), the intersection with the basal plane (001) is a line that is expressed as

$$\frac{x}{\frac{1}{h}} + \frac{y}{\frac{1}{k}} = 1$$

Where we set the lattice constant a =b=1 in the hexagonal lattice for simplicity.

Therefore the line equation becomes

hx+ky =1

The line along the $\hat{u}$ axis can be expressed as

x=y

The intersection point of the two lines occurs at the point [1/(h+k), 1/(h+k)]

The vector from origin to the point can be expressed along the $\hat{u}$ axis as

$$\mathrm{x}\hat{\mathrm{x}} + \mathrm{y}\hat{\mathrm{y}} = \frac{1}{\mathrm{h}+\mathrm{k}}\hat{\mathrm{x}} + \frac{1}{\mathrm{h}+\mathrm{k}}\hat{\mathrm{y}} = \frac{1}{\mathrm{h}+\mathrm{k}}(\hat{\mathrm{x}} + \hat{\mathrm{y}}) = \frac{1}{-(\mathrm{h}+\mathrm{k})}\hat{\mathrm{u}}$$

In other words, according to the definition

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

(c) Transformation from Miller [xyz] to Miller-Bravais index [hkil]

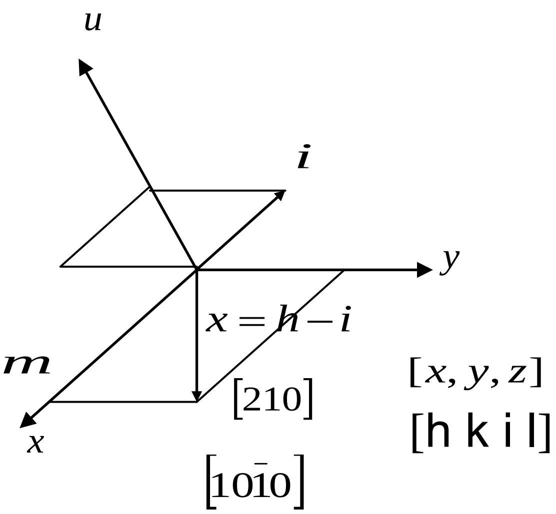
rule :

$$h = \frac{2x-y}{3}$$

$$k = \frac{2y-x}{3}$$

$$i = \frac{-(x+y)}{3}$$

$$z = l$$



Proof:

The same vector is expressed as [xyz] in miller indices and as [hkil] in Miller-Bravais indices

Therefore,

$$[xyz] = x\hat{x} + y\hat{y} + z\hat{z}$$

$$[hkil] = h\hat{x} + k\hat{y} + i\hat{u} + l\hat{z}$$

$$[hkil] = h\hat{x} + k\hat{y} + i(-\hat{x} - \hat{y}) + l\hat{z}$$

$$[hkil] = (h - i)\hat{x} + (k - i)\hat{y} + l\hat{z}$$

x = h - i

y = k - i

z = l

Moreover, h + k = - i

We can obtain

x = h – i = h +h + k $\Rightarrow$ x = 2h +k

y = k – i = k + h + k $\Rightarrow$ y = h +2k

$$h = \frac{2x - y}{3}$$

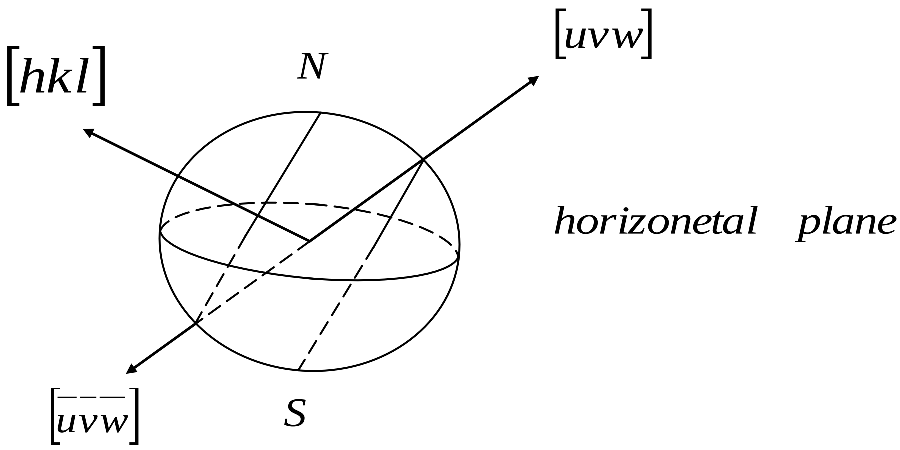
$$k = \frac{2y - x}{3}$$

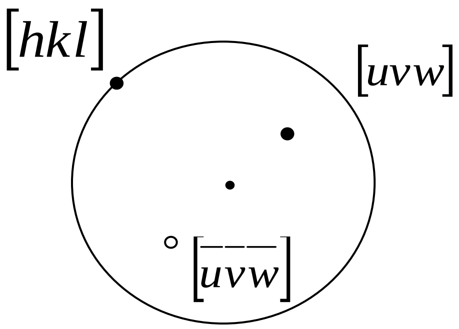
$$i = \frac{-(x + y)}{3}$$

$$z = l$$

2-4 Stereographic projections

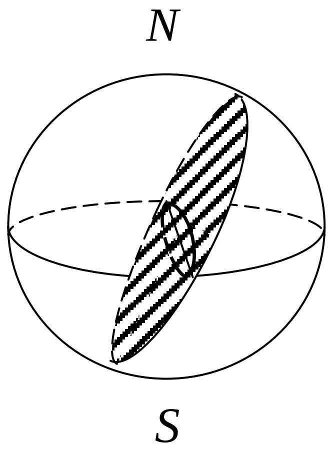
2-4-1 direction

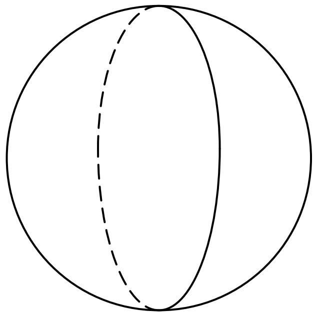




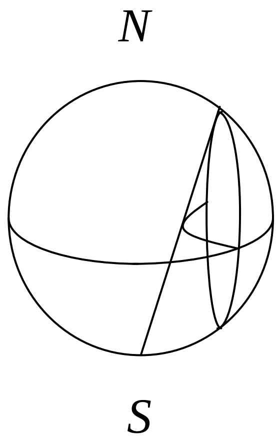
2-4-2 plane

Great circle: the plane passing through the center of the sphere.



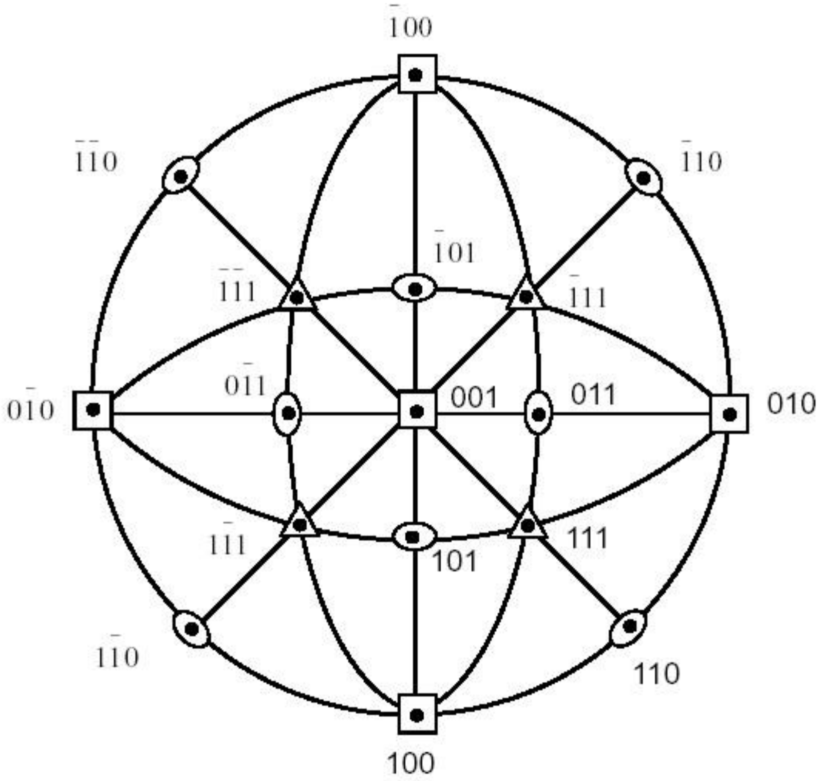


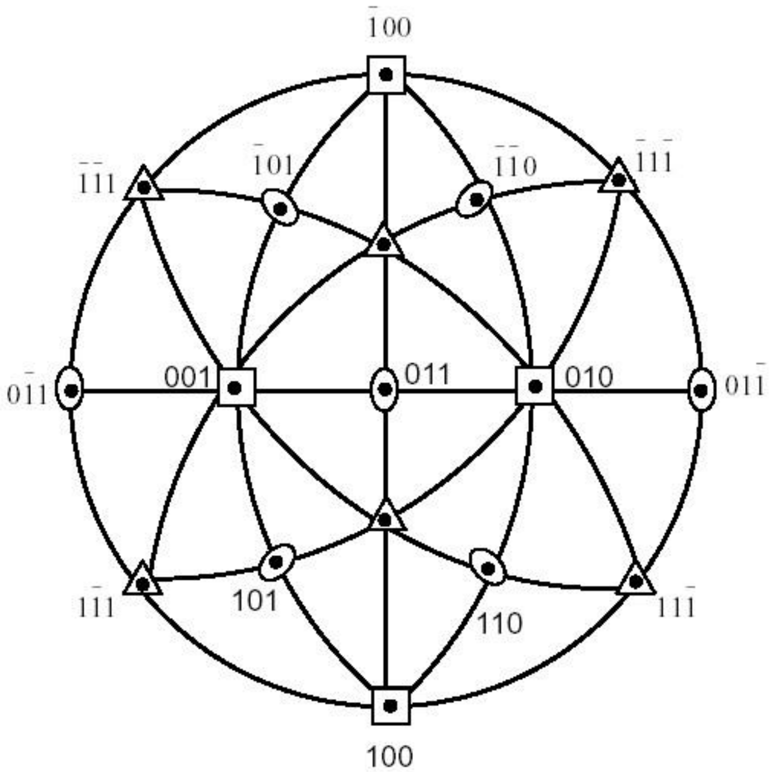
Small circle: the plane not passing through the center of the sphere.



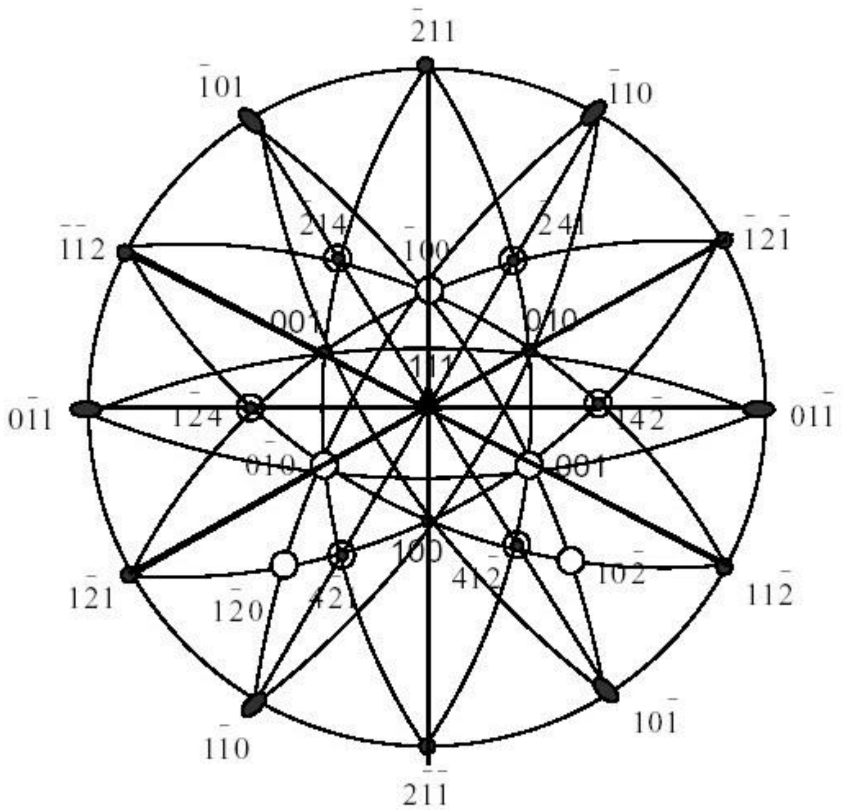
2-4-3 Stereographic projection of different Bravais systems

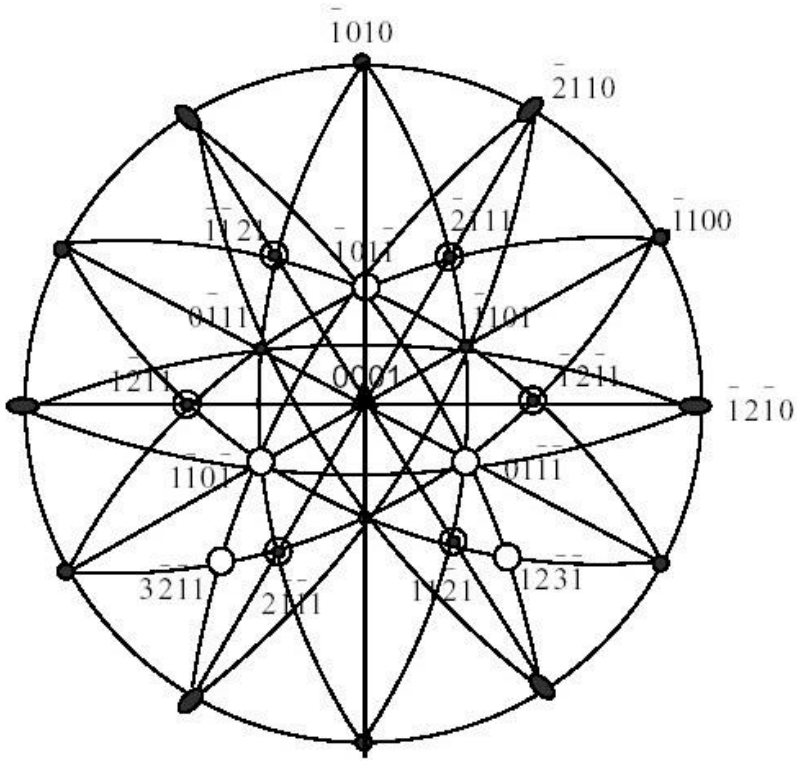
Cubic



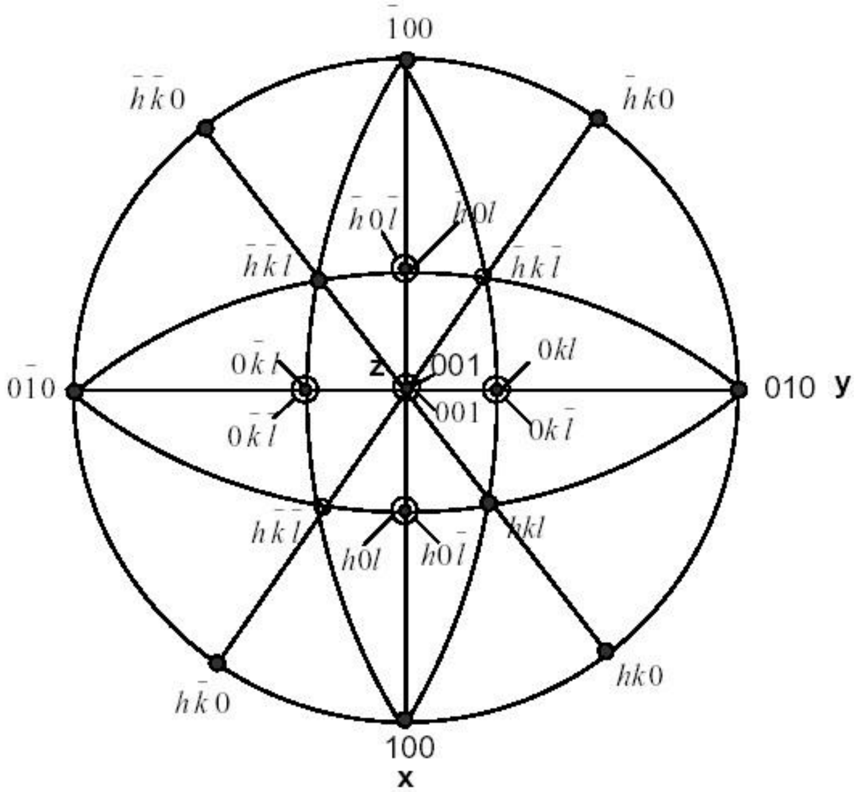


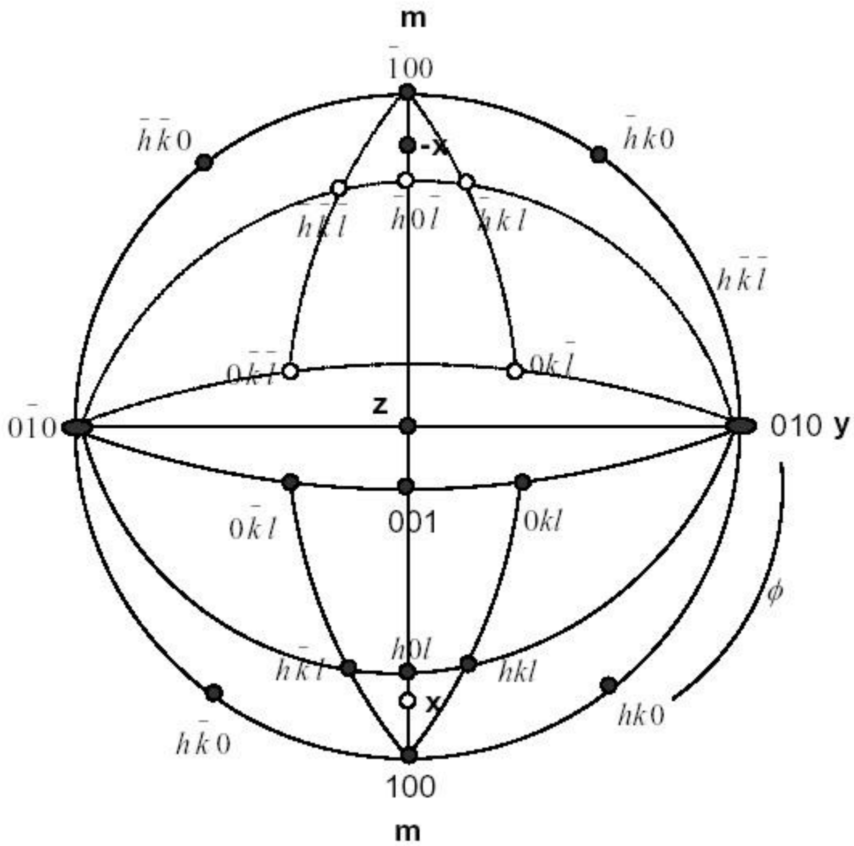
Trigonal and Hexagonal





Orthorhombic and Monoclinic



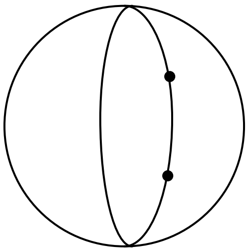


2-5 Two convections used in stereographic projection

(1) plot directions as poles and planes as great circles

(2) plot planes as poles and directions as great circles

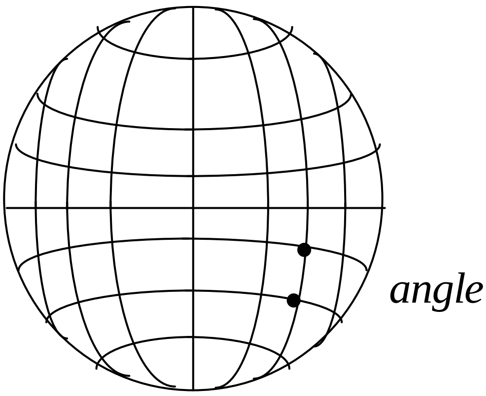
2-5-1 find angle between two directions



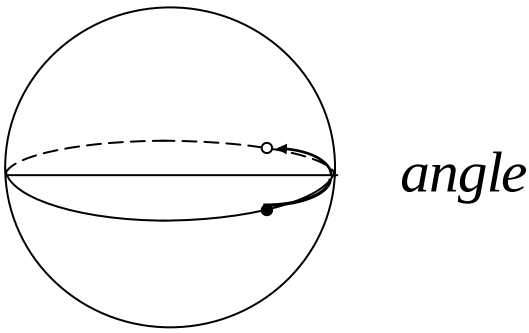
(a) find a great circle going through them

(b) measure angle by Wulff net

(i) If two poles up



(ii) If one pole up, one pole down



2-5-2 measuring the angle between planes

This is equivalent to measuring angle between poles

> use of stereographic projections

(i) plot directions as poles

---- used to measure angle between directions

---- use to establish if direction lie in a particular plane

(ii) plot planes as poles

---- used to measure angles between planes

---- used to find if planes lies in the same zone