Crystal Directions and Crystal Planes: Miller Indices

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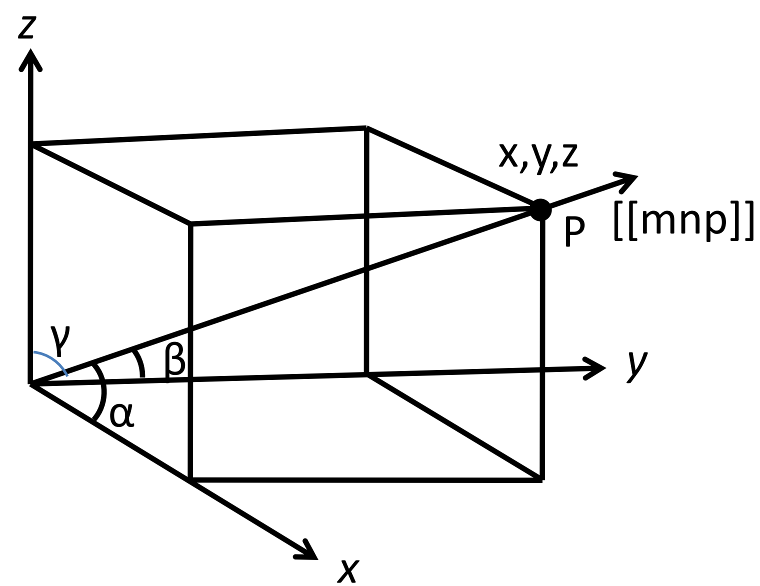
Miller Indices

A notation conventionally used to describe lattice points(sites), directions and planes is known as Miller indices.

Site Indices**:** Position of any lattice site with respect of a selected origin is defined by three of its coordinates expressed as m**a**,n**b**,p**c**.

Taking lattice parameters **a**,**b**,**c** as unit translations, the lattice coordinates are m, n, p. These numbers are site indices represented by [[mnp]].



For negative index a bar is written above the index.

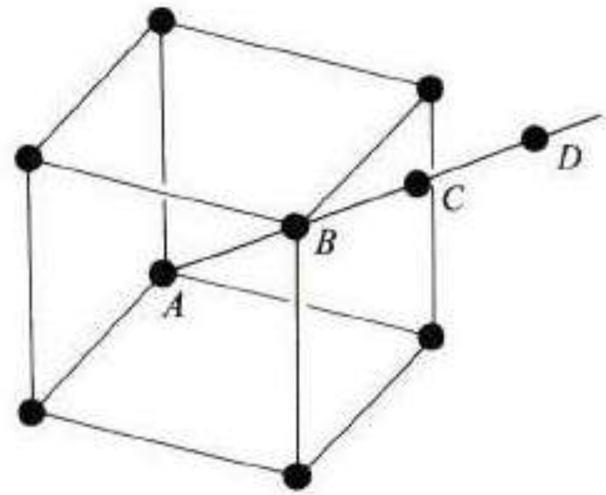
x= − 3a,y=−2b,z=1c, the site indices are written as $[[\bar{3}\ \bar{2}\ 1]]$

Crystal Direction

To specify any lattice direction we choose one lattice point on the line as an origin, say the point A. Then we choose the lattice vector joining A to any point on the line, say point B. This vector can be written as

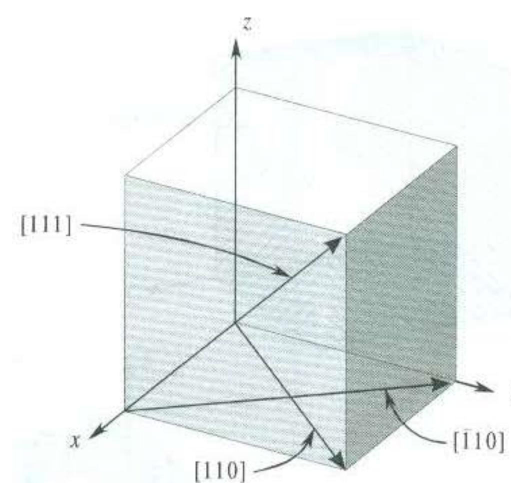
$\mathbf{R} = n_1\mathbf{a}+n_2\mathbf{b}+n_3\mathbf{c}$

The direction is specified by the integral multiplet [n_1 n_2 n_3]. The common factor is removed and the triplet is the smallest integer with same relative ratio.



[1 1 1] direction in a cubic lattice

Due to rotational symmetry some non parallel directions are equivalent and represented as <n_1 n_2 n_3>



Crystal Planes and Miller indices

The equation of a plane having intercepts *p*, *q*, *r* with the *x*, *y*, *z* axes is given by

$$\frac{x}{p}+\frac{y}{q}+\frac{z}{r}=1$$

•Determine the intercepts of a plane with the axes along the basis vectors ***a***, ***b***, ***c***.

•The intercepts *p****a***, *q****b***, *r****c*** is divided by the unit basis vectors ***a***, ***b***, ***c***.

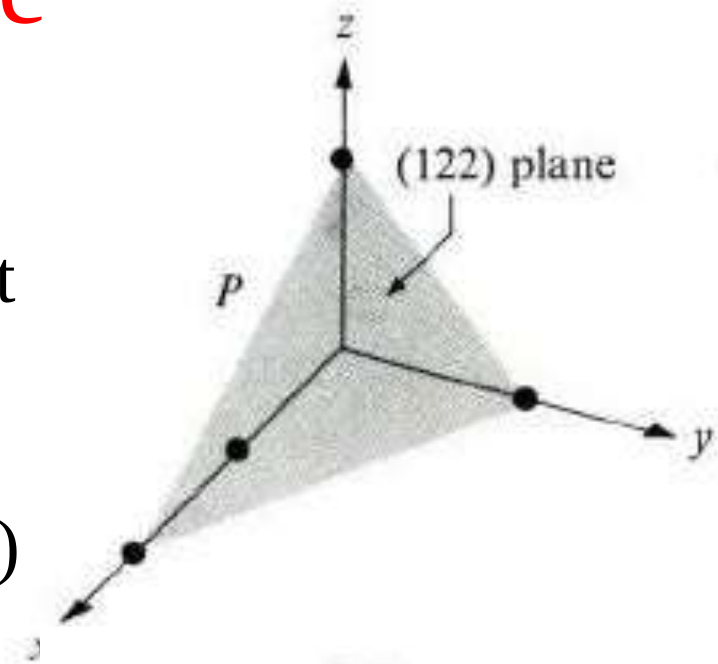
•Take the reciprocal to form a triplet (*1/p*,*1/q/*,*1/r*).

•Reduce it to a similar one having the smallest integers by multiplying by a common factor.

• Put the resulting integers in parenthesis as (*hkl*), which is the required Miller Indices and represents all the parallel planes.

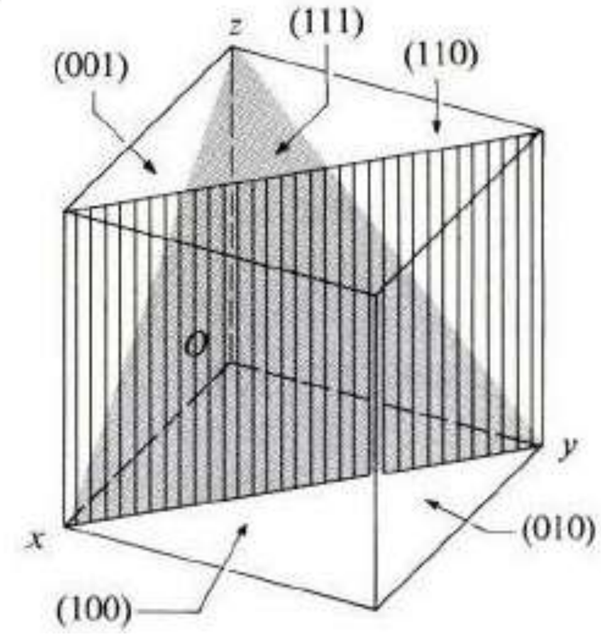
Example

- Intercepts are 2a, 1b, 1c
- Divide by unit basis vectors to get (2,1,1)
- Take reciprocal (1/2,1,1)
- Convert to smallest integer (1 2 2)



Assignment:

Check the validity of planes shown



Representation of Planes of known Miller Indices

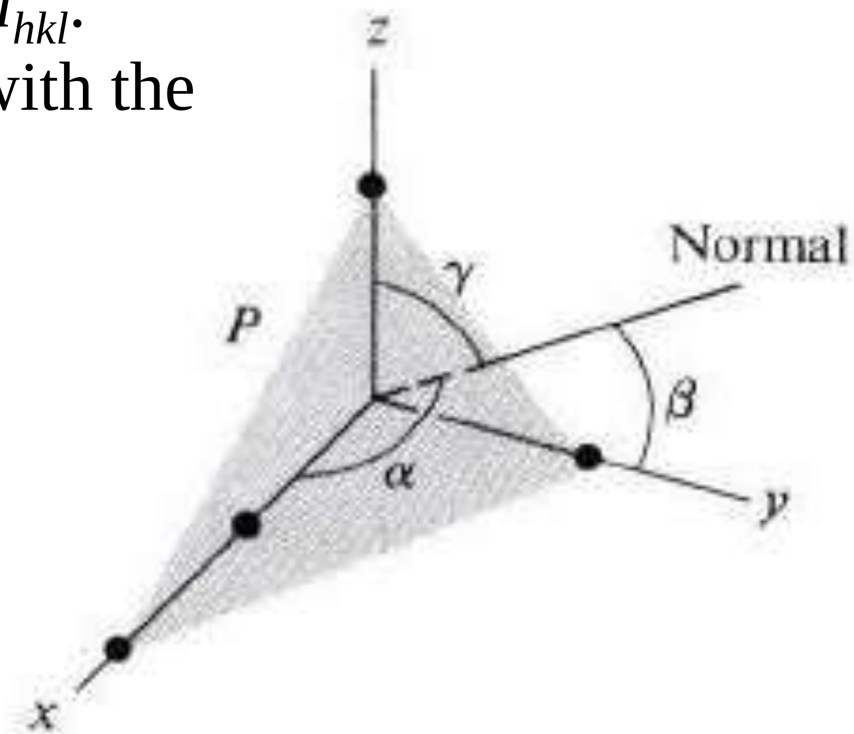
- Take reciprocal of the given Miller Indices. They represent intercepts in terms of basis vectors.
- Mark the length of intercepts on the respective axes. Join the end points, the resulting sketch will represent the required plane.

Representation Family of Planes

- When the unit cell has rotational symmetry, several nonparallel planes may be equivalent by virtue of this symmetry.
- All these planes are lumped in the same Miller indices, but with curly brackets.
- The indices {*hkl*} represent all the planes equivalent to the plane (*hkl*) through rotational symmetry.
- In the cubic system the indices {100} refer to the six planes (100), (010), (001),($\bar{1}00$), ($0\bar{1}0$), and ($00\bar{1}$)

Spacing Between Planes of Same Miller Indices

The interplanar spacing is given by d_{hkl}.
The normal makes angle α, β and γ with the axes.
The intercepts on the axes are x, y, z.



$$d_{hkl} = x\cos\alpha = y\cos\beta = z\cos\gamma$$

$$\cos^2\alpha + \cos^2\beta + \cos^2\gamma = 1$$

$$d_{hkl} = \frac{1}{\left(\frac{1}{x^2} + \frac{1}{y^2} + \frac{1}{z^2}\right)^{\frac{1}{2}}}$$

$$h = \frac{a}{x}, k = \frac{b}{y}, l = \frac{c}{z}$$

$$d_{hkl} = \left(\frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}\right)^{-\frac{1}{2}}$$

Thank You

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