Miller Indices

Definition

- Miller indices are used to specify directions and planes.
- These directions and planes could be in lattices or in crystals.
- The number of indices will match with the dimension of the lattice or the crystal.
- E.g. in 1D there will be 1 index and 2D there will be two indices etc.

Notation Summary

- (h,k,l) represents a point – note the exclusive use of commas
- (hkl) represents a plane.
- [hkl] represents a direction

Miller Indices for Directions

- A vector r passing from the origin to a lattice point can be written as:

  $r = r_1a + r_2b + r_3c$

- where, a, b, c → basic vectors and miller indices → $(r_1r_2r_3)$
- Fractions in $(r_1r_2r_3)$ are eliminated by multiplying all components by their common denominator.

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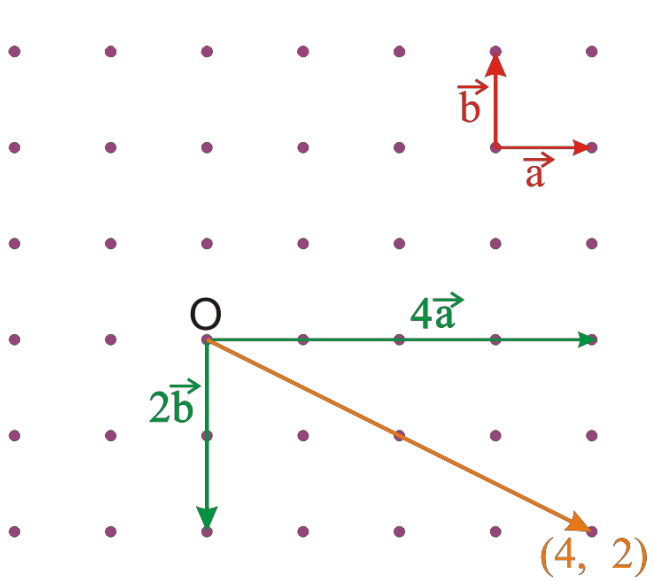
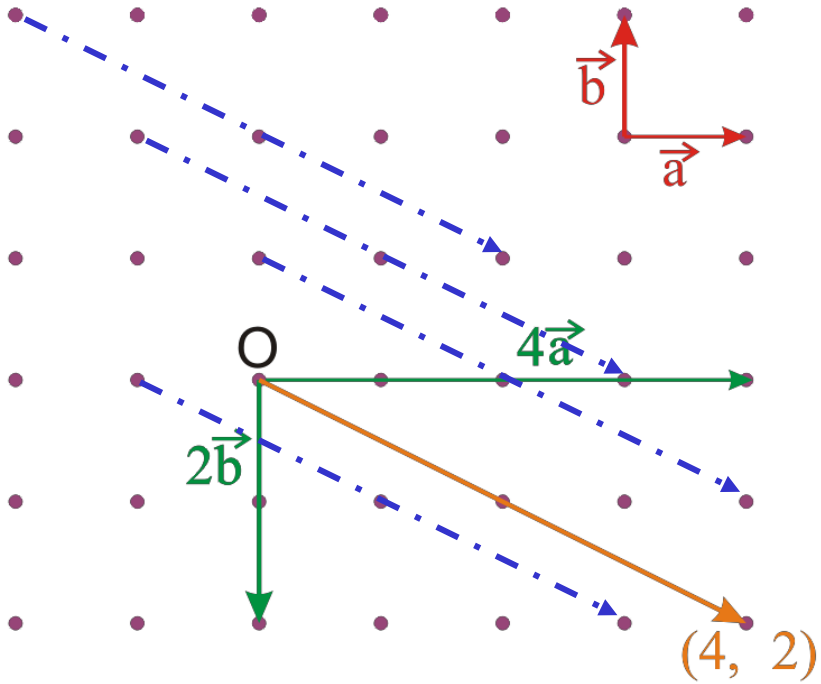


Miller indices = [42]



The index represents a set of all such parallel vectors

Indexing planes in a lattice

- **Miller Index**: Reciprocal of intercepts a plane makes on the crystallographic unit cell axes
- **Step 1** : *Identify the intercepts on the x- , y- and z- axes.*
- The intercept on the x-axis is at $x = a$ (at the point (a,0,0)), but the surface is parallel to the *y*- and *z*-axes. That is, there is no intercept on these two axes. Therefore, the intercept has to be at infinity (∞) for the case where the plane is parallel to an axis.

  The intercepts on the *x*- , *y*- and *z*-axes are thus Intercepts : ($\boldsymbol{a , \infty , \infty}$)

- **Step 2** : *Specify the intercepts in fractional co-ordinates*
- Co-ordinates are converted to fractional co-ordinates by dividing by the respective cell-dimension - for example, a point (x,y,z) in a unit cell of dimensions $a \times b \times c$ has fractional co-ordinates of (x/a , y/b , z/c). In the case of a cubic unit cell each co-ordinate will simply be divided by the cubic cell constant , a . This gives fractional Intercepts : $\boldsymbol{a/a , \infty/a, \infty/a}$ i.e. $\boldsymbol{1 , \infty , \infty}$

- **Step 3** : *Take the reciprocals of the fractional intercepts*
- This final manipulation generates the Miller Indices which (by convention) should then be specified without being separated by any commas or other symbols. The Miller Indices are also enclosed within standard brackets (….) when one is specifying a unique surface.
- The reciprocals of **1** and ∞ are **1** and **0** respectively, thus yielding **Miller Indices** : **(100)** (see next page)

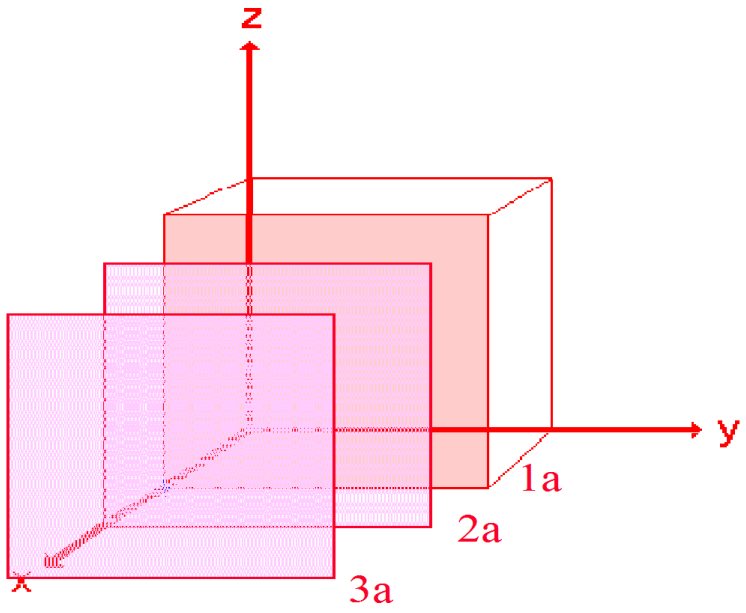
Miller Indices for Planes:

Procedure

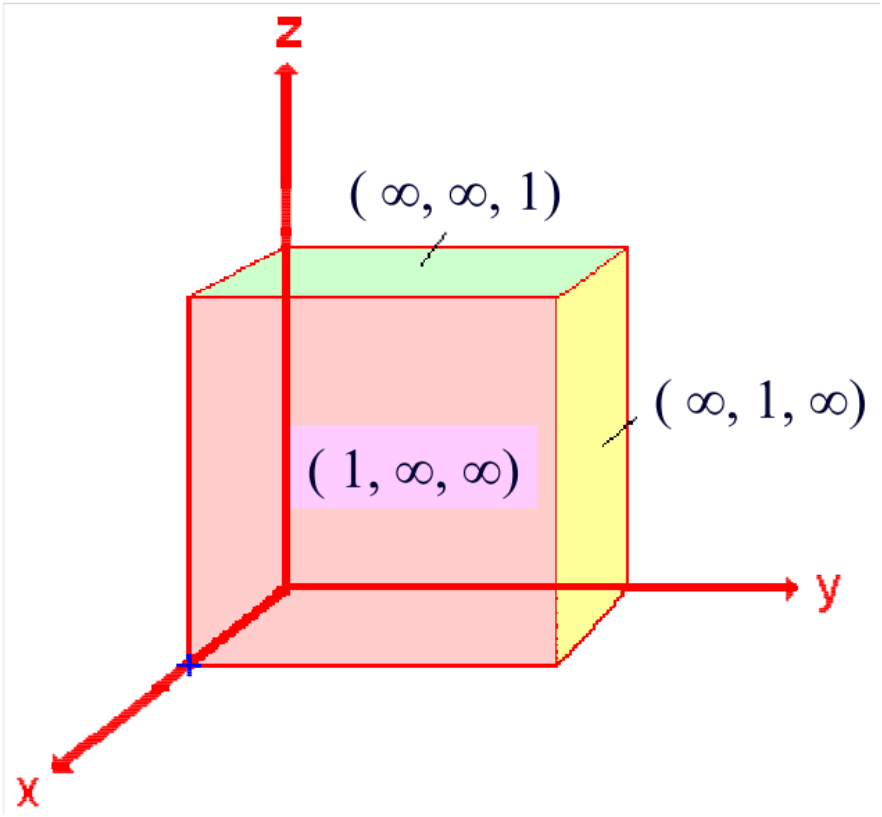
- ❑ **Identify the plane intercepts on the x, y and z-axes.**
- ❑ **Specify intercepts in fractional coordinates.**
- ❑ **Take the reciprocals of the fractional intercepts.**

Miller Indices for Planes: Illustration

• Consider the plane in pink, which is one of an infinite number of parallel plane each a consistent distance (“a”) away from the origin. (purple planes)



- The plane intersects the x-axis at point a. It runs parallel along y and z axes.
- Thus, this plane can be designated as (1,∞, ∞)



- Likewise, the yellow plane can be designated as (∞,1,∞)
- And the green plane can be written as (∞,∞,1)

Miller Indices are the reciprocals of the parameters of each crystal face. Thus:

- Pink Face

  = (1/1, 1/∞, 1/∞) = (100)

- Green Face

  = (1/∞, 1/∞, 1/1) = (001)

- Yellow Face

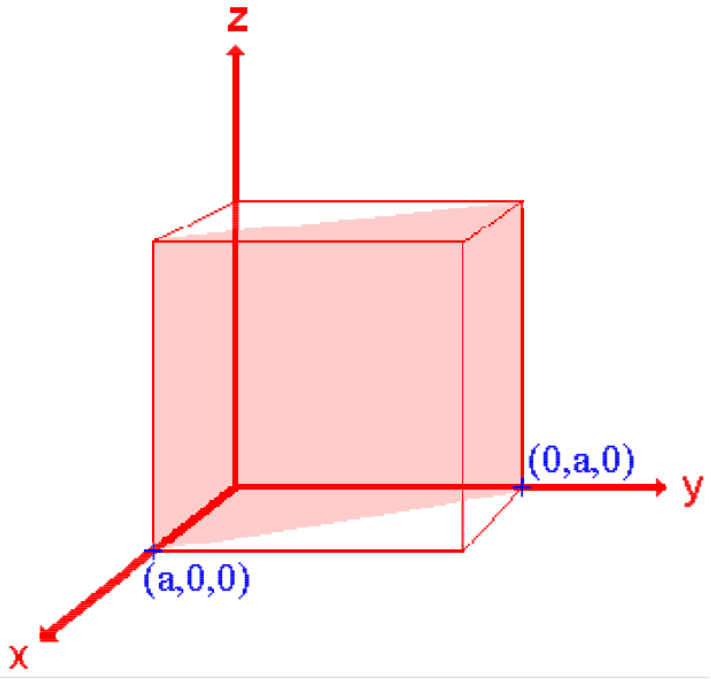
  = (1/∞, 1/1, 1/∞) = (010)

Examples

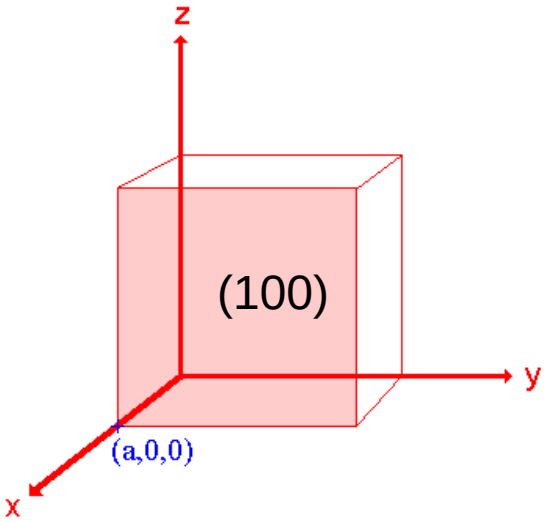
Miller Indices

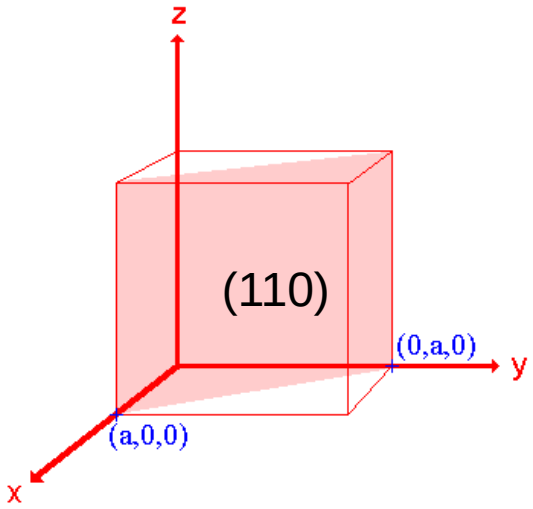
What's the Miller Index of this plane?

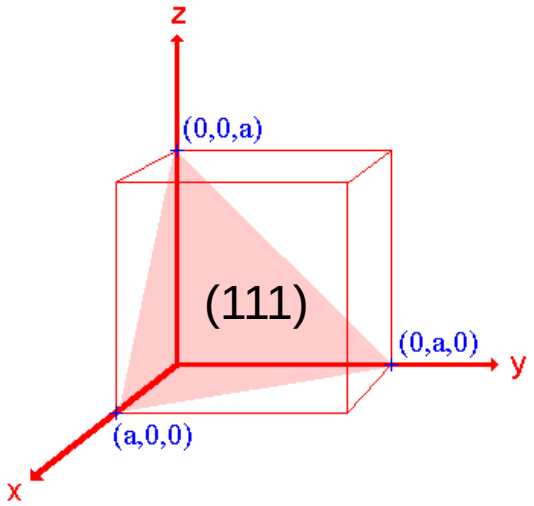
The plane of interest cuts two of the crystallographic Intercepts: (1,1, ∞) → (110)



Crystallographic planes



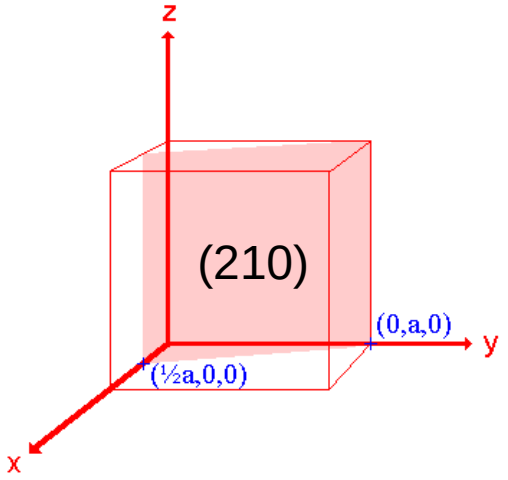




Miller indices are **(hkl)** values.

[hkl] means directions perpendicular to the **(hkl)** plane from the origin

Assignment: Construct the planes with the following Miller indices in a cubic lattice: (101), (120), (321), (412), (043), (303)



This plane cuts two of the reference axes, but not equidimensionally.

- **Tricky; this plane cuts two of the crystallographic axes, but not equidimensionally**
- **Intercepts: (½, 1, 0) → (210)**

Interplanar Spacing

The perpendicular spacing **(d spacing)** between parallel planes **(Miller indices *hkl*)** may be calculated using the following equations.

Cubic $$\frac{1}{d^2} = \frac{h^2 + k^2 + l^2}{a^2}$$

Tetragonal $$\frac{1}{d^2} = \frac{h^2 + k^2}{a^2} + \frac{l^2}{c^2}$$

Orthorhombic $$\frac{1}{d^2} = \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}$$

Lattice planes and d-spacing

- Relationship between lattice planes and d- spacing for an orthorhombic crystal system with unit cell parameter *a*,*b* & *c*.
- $\frac{1}{d_{hkl}^2} = \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}$
- Relationship between lattice planes and d- spacing for a cubic crystal system with unit cell parameter '*a*'.
- $\frac{1}{d_{hkl}} = \frac{\sqrt{h^2+k^2+l^2}}{a}$
- For first order diffraction, $n\lambda = 2d \sin\theta$ where n=1
- Also the expression for density of the a crystalline sample is given by
- $\rho = \frac{nM}{N_A V}$ where 'ρ' is the density, '*n*' is the number of molecules /ions per unit cell, N_A is the Avogadro's number and '*V*' is the Volume of the unit cell.
- For cubic system $V = a^3$, where is the edge length.
- For orthorhombic system $V = a \times b \times c$, where *a*, *b* and *c* are unit cell edges

- **Obtain the *d*-spacing for the lattice planes with miller indices (111), (210), (121), (320), (321) a) for a cubic lattice with *a*= 3.0Å**
  and b) an orthorhombic lattice with *a* = 2.0Å, *b*=3.0Å and *c* = 4.0Å.

Example:

For Cubic lattice with a =3.0Å

d-spacing for the lattice plane with miller indices (210)

$$\frac{1}{d^2} = \frac{h^2 + k^2 + l^2}{a^2}$$

h= 2, k=1, l=0

$1/d^2 = (4+1+0)/9$ Å^2

$d^2 = 1.8$ Å

$= 1.34$ Å

- **At room temperature Po crystallises in Primitive cubic system with *a*= 3.36Å. Calculate density if the At. Wt. of Po is 209g/mol**

- **$LiBH_4$ crystallises in orthorhombic system with 4 molecules per unit cell. Calculate the density if M.Wt. is 21.76g/mol and the cell parameters *a* = 6.81Å, *b* = 4.43Å, *c* = 7.17Å**