Miller indices and Family of the Planes

The geometrical features of the crystals represented by lattice points are called **Rational.** Thus a lattice point (or site in lattice) with respect to another lattice point is called **Rational Point.** A row of lattice point is called **Ration Line** and the the a plane defined by (rational) lattice point is called **Rational Plane.** All other features are called **Irrational Features**.

It is necessary to have an appropriate notations to describe the rational features. A notation used for describing these rational features (point, line and plane) is called **Miller Indices.**

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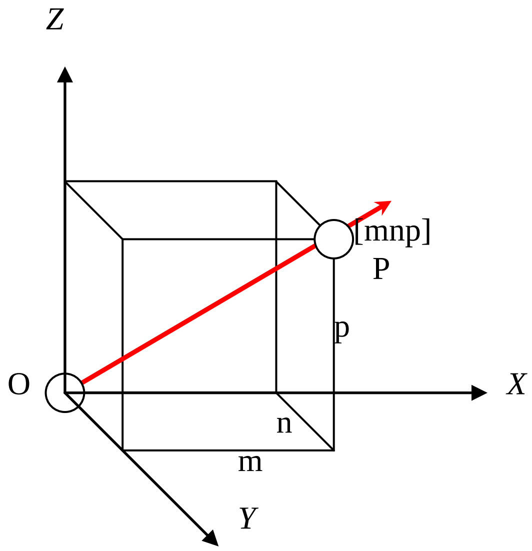
Indices for point or site indices

A position of a point or site in the lattice is always described with respect to arbitrarily



chosen one of the lattice point as an origin and representing it in terms of cartisian coordinates. These coordinates are expressed in the following forms; x=ma, y=nb, and z=pc. Where a,b, and c are lattice constant and m,n, and p are integers. The cite indices of the point P is [[mnp]]. For the negative indices the 'bar' is written over the index. For the site with the coordinates x = -2a, y =1b and z=-3c, the site indices are written as [[$\bar{2}1\bar{3}$]] **<u>Problem: Determine the indices of the sites depicted in the two dimensional net.</u>**

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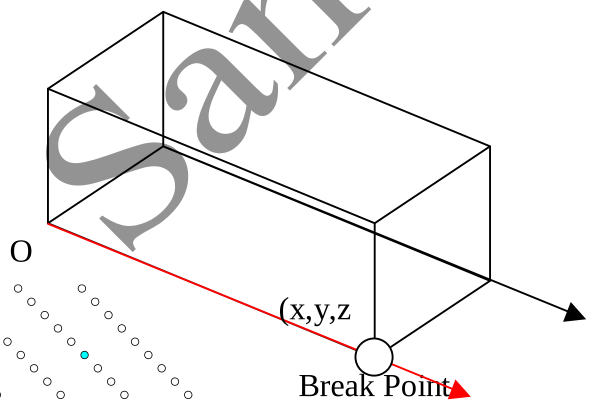
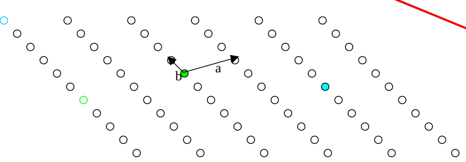
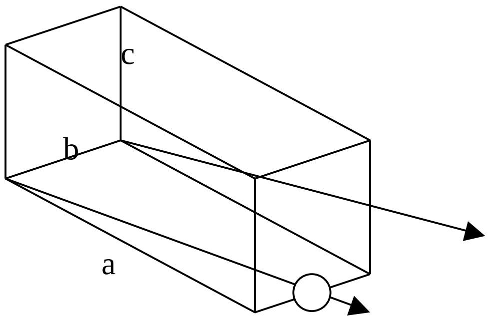
Indices of Direction:



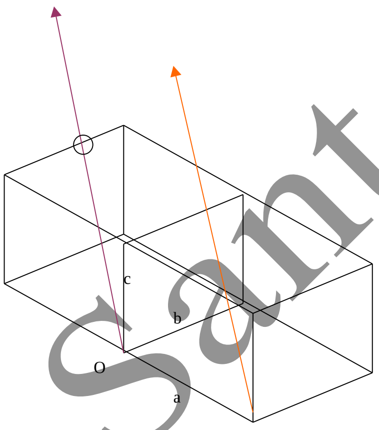


To describe a direction in crystal lattice, a straight line passing through origin and parallel to the line of direction under the investigation is drawn. Then the coordinates of a point through which the chosen line emerge out or 'break open' the unit cell is determined. The coordinates of the ‘break open’ point in the given example is 1,0,0 in terms of a,b, and c respectively. It is indicated by [100]. The same line will also pass through (2x 2y 2z), (3x 3y 3z), (4x 4y 4z)…….and will have common coordinates [x y z].

The x,y and z are arranged to be set of smallest possible integer, by dividing and multiplying through common factor.



e.g. The coordinates of the break open point is (1,1/2,0). Multiplying by 2 to all the numbers, the set of smallest possible integers is (2,1,0) and the miller indices are [210], [210], [420], [630] will havesame direction and all will desribed by the set of smallest possible intergers i.e. [210].



The coordinates of the break open points is (-1, 0.66, 1) or (-1,2/3,1). Multiply this by ‘3’ leads to coordinates (-3,2,3) thus the Miller indices are $[\bar{3}23]$

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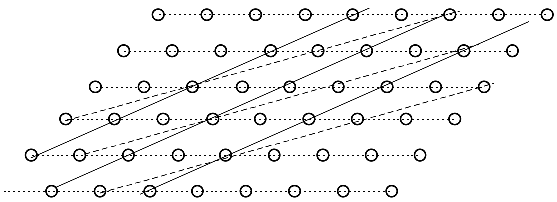
Miller indices for lattice plane

W hen we shine a X-ray radiation on a crystal, it is observed that the X-rays scatters selectively at particular direction. These anisotropic scattering of X-rays from the crystal, force us to believe a presence of atomic planes (though hypothetical) in the crystals which are oriented in the particular direction, and act as a mirror to reflect the x-ray at particular direction. Such reflecting planes are termed as **lattice planes.** **Thus Lattice planes are just imaginary equidistant surfaces on which most of the lattice points are lying.**

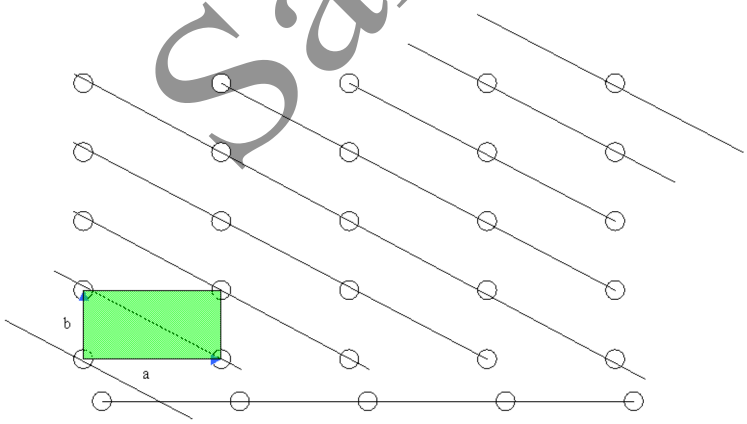


We can start with two dimensional lattice i.e. NET. In this case, The plane is just substituted by a line. One can draw infinite such lines characterized by the perpendicular distance between the two planes for a given set of plane called interplanner spacing designated by ‘d’. Some times, it also called *d-spacing*. We can give some rational names to these family of plan

es called **Miller indices.**

We will start with simple two dimensional example which will extrapolate to three dimension.

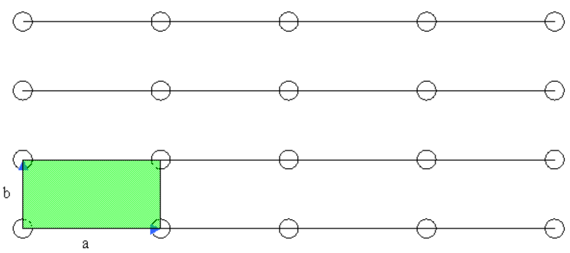
Consider the two dimensional rectangular lattice Here we have chosen set of plane passing through the lattic points. In order the determine the Miller indices,



- First chose the arbitr

ary origin and the unit cell such that one planes from the set is lying on the origin

- Then determine the intercept of the very next plane of the set



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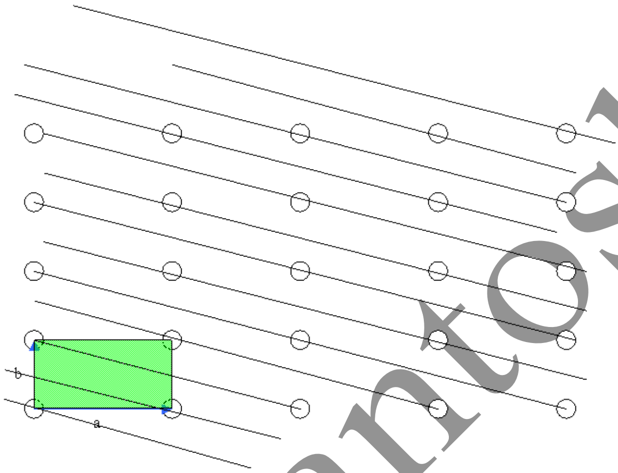
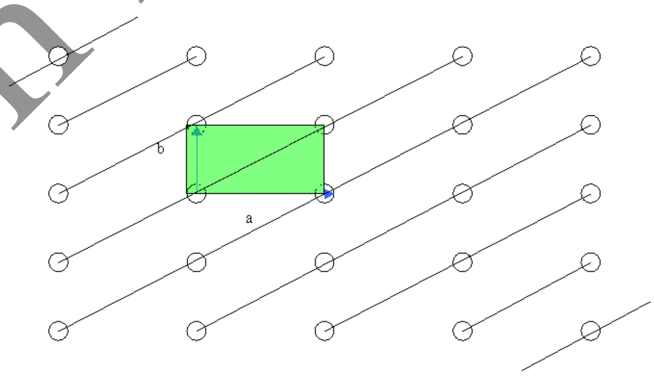
on x and y axes in terms of the unit lengths a and b respectively. The intercepts are 1a and 1b divide this number by respective unit lengths i.e. a and b

- $\frac{1a}{a}=1$ and $\frac{1b}{b}=1$

- The last step is to take reciprocal of the number . Thus, the miller indices of the plane is (1 1)

e.g. The coordinate are ∞ a and 1b deviding by a and b the intecepts are ∞ and 1 receptively , taking the reciprocal of the number (0 1)





Intercept 1a and 1/2b Therfore miller indices are (21)

In the third example, the intercept next to the plane passing through origin is 1 and –1 there fore the indices are $(1\bar{1})$ If we consider the another plane, the indices would have been $(\bar{1}\ 1)$ These two set of planes are equivalent and designated by symbol $\{\bar{1}\ 1\}$.

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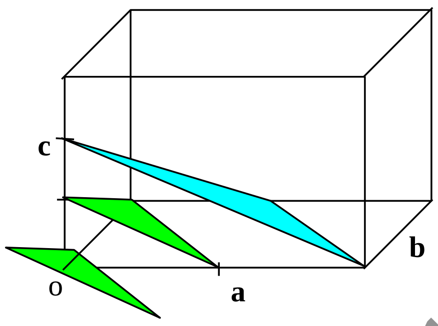
Miller indices in three Dimensional Lattice

Consider the following example.. Here point O is the chosen origin of the unit cell and a set of planes passing through the unit cell. In order to determine the miller indices of a chosen set of plane, the first step is to determine a member of set which passes through origin. After identifying such plane, determine the intercept of an immediate neighbor to all three chosen axis in terms of **a,b and c.** In a given example plane cuts the **'a'** at a/2. It cuts to b axis at 1 and c axis at c/3. The intercepts are therefore, 1/2, 1, 1/3.



Third step is to take reciprocal of all three numbers. Those would be 2,1,3. These are conventionally depicted as (213) Threrefore, the miller indices of chosen set of plane is (213). This set of plan has characteristics d value which is depicted as $d_{213.}$ The symbol, { } is used to indicate the set of planes which are equivalent. Eg. The set (100), (010) and (001) are equivalent at represented as {100}.

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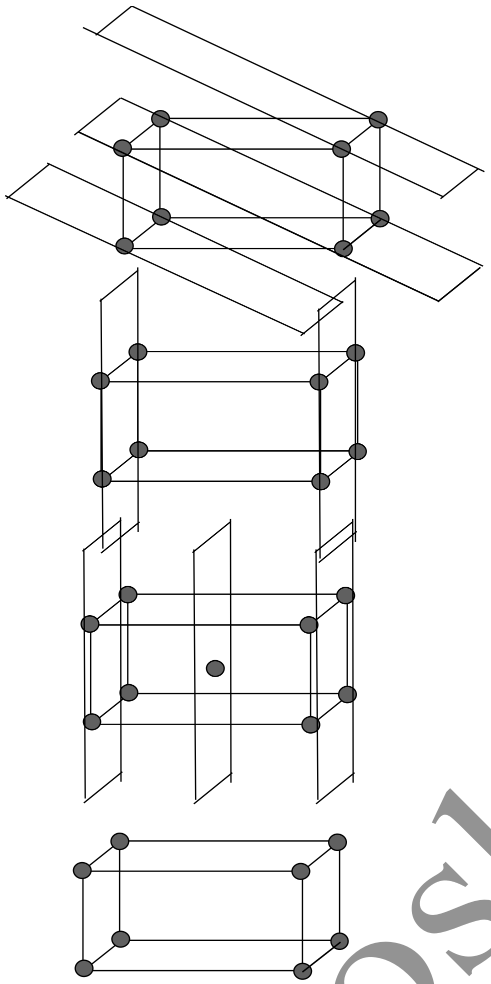

Examples: Determine The miller indices of the following lattice:

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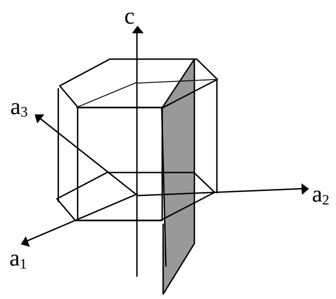
The Miller indices of Hexagonal Lattice. or Miller-Bravais indices

As discussed above, for all crystal systems, three no-coplanner axes are sufficient to describe the miller indices of the plane. However, the hexagonal unit cell are an exceptions to it. Four indices are often used for that purpose, namely (hkil). Instead of three axes, four axes are used namely, a_1 , $a_{2,}$ a_3 and c. For example, the plane which is shown in the figure cuts a_1 axis at (-1), a_2



axis at 1/2, a_3 axis at (-1) and c axis at infinite. Therefore the miller indices are ($\bar{1}$ 2 $\bar{1}$ 0)

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PROBLEMS

1. In a crystal, a plane cuts intercepts of 2a 3b and 6c along the three crystallographic axes, Determine the miller indices of the plane.

Intercept	2a	3b	6c
Division by lattice constants	2a/a=2	3b/b=3	6c/c=6
Reciprocal	½	1/3	1/6
After clearing fractions (multiply by 6)	3	2	1
Miller indices	(321)		

2. Determine the Miller indices of a plane which is parallel to the x-axis and cuts intercepts of 2 and ½, respectively along y and z axes.

Intercept	∞a	2b	1/2c
Division by lattice constants	∞a/a=∞	2b/b=2	1/2c/c=1/2
Reciprocal	0	½	2
After clearing fractions (multiply by 2)	0	1	4
Miller indices	(014)		

3 An orthorhombic Crystal whose primitive translations are a= 1.21A, b=1.84A and C=1.97A respectively. If plane of miller indices $(23\bar{1})$ cuts an intercept of 1.21A along 'x' axis find the length of intercept at 'y' and 'z' axes.

h:k:l =2:3:$\bar{1}$

Ratios of the intercepts would be $\frac{1.21}{2} : \frac{1.84}{3} :-1.97$

Now its cuts at x axis at 1.21A, then obviously we have to multiply all the numbers by 2 and we get 1.21:1.22:-3.94

Answer: it will intercept at 1.22A and –3.94A at y and z axes respectively.

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4.The distance between the consecutive (111) plane in a cubic crystal is 2A determine the lattice parameter.

Solution:

For the cubic crystals, we have

$$d = \frac{a}{\sqrt{h^2+k^2+l^2}} = \frac{2}{\sqrt{1+1+1}} = \frac{2}{\sqrt{3}} A$$

5. In the teragonal crystal, the lattice parameter a=b=2.42A and c=1.74A, determine the inteplanner spacing between consecutive (101) planes

Solution: For the tetragonal cell,

$$\frac{1}{d^2} = \frac{h^2+k^2}{a^2} + \frac{l^2}{c^2} = \frac{1+0}{2.42^2} + \frac{1}{1.74^2} =$$

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