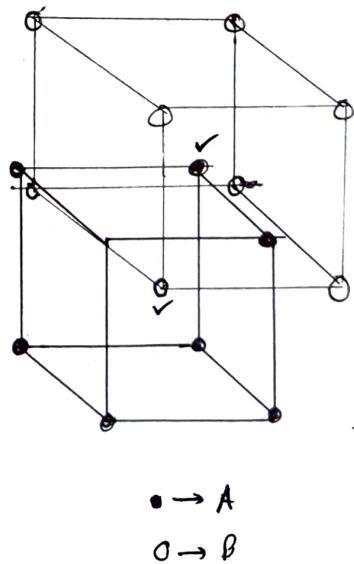


## Lecture 6

2

Although we have discussed about the fourteen Bravais lattices, let's talk a bit about the few important and most occurring ones of them. Also, it is not always evident that all the lattice points are actually equivalent. Let's see examples emphasizing this fact.

Consider a body-centered cubic (bcc) lattice. We will form this lattice by adding an additional point at the center of a simple cubic lattice (whose sites are now A). However, the center atom is part of another simple cubic lattice whose sites are given by B. In BCC lattice, one might feel that the center point bears different relations than the points at the corners. However, as shown here, the center atom B in the SC lattice made from A here, is the corner point of a different SC lattice, made from the same BCC lattice. Also, A acts as the center point of the SC lattice made from B points. So, if you consider



BCC lattice where corner points are A, you can make another SC lattice using the center points B of the neighboring cells. This clearly shows that the view is same from all the lattice sites.

The simple cubic lattice <sup>(side length 'a')</sup> can be generated by three primitive vectors  $\vec{a}_1 = a\hat{x}$ ,  $\vec{a}_2 = a\hat{y}$  and  $\vec{a}_3 = a\hat{z}$ . Any lattice point can then be written  $\vec{R}$  denoted by the vector  $\vec{R} = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3 = a(\hat{x} + \hat{y} + \hat{z})$   
 $= a(n_1 \hat{x} + n_2 \hat{y} + n_3 \hat{z})$

For the BCC lattice, we can take  $\vec{a}_1 = a\hat{x}$ ,  $\vec{a}_2 = a\hat{y}$  and  $\vec{a}_3 = \frac{1}{2}a(\hat{x} + \hat{y} + \hat{z})$ . According to this choice,

$$A = (0, -1, 2), D(-1, -1, 2), B(0, 0, 2), C(-1, 0, 2)$$

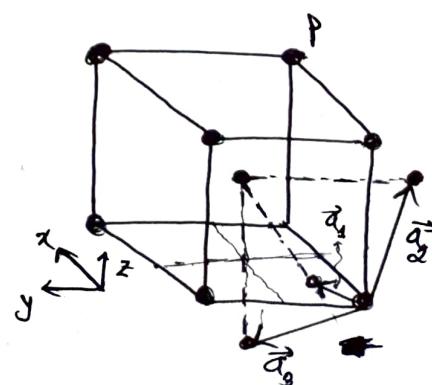
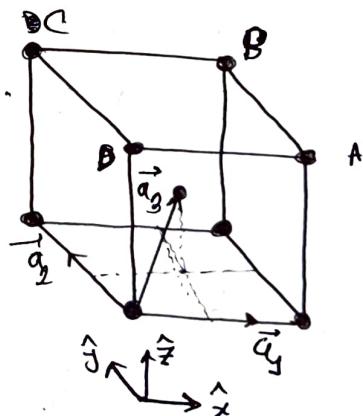
One can express the whole BCC lattice in the form of  $\vec{R} = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3$  to find all the lattice points.

Another possible choice might

$$\vec{a}_1 = \frac{1}{2}a(-\hat{x} + \hat{y} + \hat{z})$$

$$\vec{a}_2 = \frac{1}{2}a(\hat{x} - \hat{y} + \hat{z})$$

$$\vec{a}_3 = \frac{1}{2}a(\hat{x} + \hat{y} - \hat{z})$$



where the  $n$  points are basically the <sup>three</sup>  $\nwarrow$  center points near a corner point (origin). One can easily find the position in the Cartesian coordinate, and then find the values of  $n_1, n_2$  and  $n_3$  by solving three linear equations. For example, if you want to express the position of point  $P$  using these bases, the followings are the steps.

In Cartesian coordinates,  $P = P(a, 0, a)$

$$\vec{R}_P = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3 = \frac{a}{2} (-n_1 \hat{x} + n_2 \hat{y} + n_3 \hat{z}) + \dots$$

$$\Rightarrow a\hat{x} + 0\hat{y} + a\hat{z} = \frac{1}{2} a [(-n_1 + n_2 + n_3) \hat{x} + (n_1 - n_2 + n_3) \hat{y} + (n_1 + n_2 - n_3) \hat{z}]$$

$$\Rightarrow \hat{x} + 0\hat{y} + \hat{z} =$$

$$\therefore (-n_1 + n_2 + n_3) \frac{a}{2} = a \quad \left| \begin{array}{l} (n_1 - n_2 + n_3) \frac{a}{2} = 0 \\ (n_1 + n_2 - n_3) \frac{a}{2} = a \end{array} \right.$$

$$\Rightarrow n_1 = n_2 + n_3 - 2 \quad \text{--- (I)}$$

$$\left| \begin{array}{l} \Rightarrow n_1 = n_2 - n_3 \quad \text{--- (II)} \\ \Rightarrow n_1 = n_3 - n_1 + 2 - n_3 \end{array} \right. \quad \Rightarrow n_2 = n_3 - n_1 + 2 \quad \text{--- (III)}$$

$$\Rightarrow n_1 = 1$$

$$\therefore (\text{III}) \Rightarrow n_2 = n_3 + 1$$

$$(I) \Rightarrow 1 = n_2 + n_3 - 2$$

$$\therefore n_2 = -n_3 + 3$$

$$\therefore n_3 + 1 = -n_3 + 3$$

$$\therefore n_3 = 1 \quad \text{and so, } \cancel{n_2} = \cancel{n_2} = 2$$

$$\therefore \vec{R}_p = \vec{a}_1 + 2\vec{a}_2 + \vec{a}_3$$

One can find the expression of  $\vec{R}$  for any point in the lattice by this manner.

Similarly, we can consider three primitive vectors as shown in the following figure. They can be written as,

$$\vec{a}_1 = \frac{a}{2}(\hat{x} + \hat{y}), \quad \vec{a}_2 = \frac{a}{2}(\hat{x} + \hat{z}) \text{ and} \\ \vec{a}_3 = \frac{a}{2}(\hat{y} + \hat{z})$$

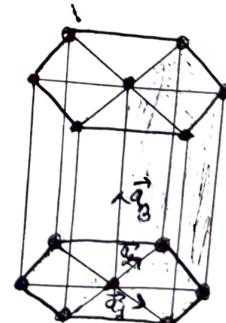
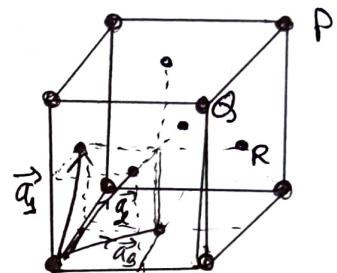
Using these basis vectors,

$$\vec{R}_p = \vec{a}_1 + \vec{a}_2 + \vec{a}_3, \quad \vec{R}_k = \vec{a}_2 + \vec{a}_3 \quad \text{and} \quad \vec{R}_g = \vec{a}_2 + \vec{a}_3 - \vec{a}_1$$

The following figure shows the primitive vectors of a hexagonal lattice. Here,  $|\vec{a}_1| = |\vec{a}_2| = a$  and  $|\vec{a}_3| = a'$ .

You can ~~not~~ express the position of each point using  $\vec{a}_1, \vec{a}_2$  and  $\vec{a}_3$ .

Note that, these primitive basis vectors creates a primitive cell, and contains precisely one point. This is evident in the hexagonal lattice. However, one can show this for bcc and fcc lattice as well (see Kittel, page 13).



## Direction and crystal planes: and Miller indices

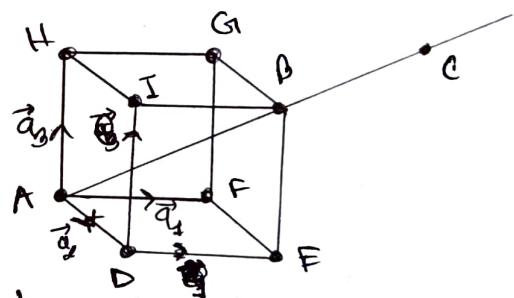
In describing the physical phenomena in crystals, we must often specify certain directions and/or crystal planes. The convention and a few examples are provided here.

### Crystal directions

Consider the straight line passing through the lattice points A, B, C etc. (AB is along the body diagonal of the lattice).

To specify the direction, we proceed as follows:

We choose a lattice point on the line (say A) as the origin. Then we choose the lattice vector joining A to any point on the line, say B. This vector can be written as,  $\vec{R} = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3$ . The direction is then specified by the integral triplet  $[n_1 n_2 n_3]$ . If the number has a common factor, the factor is removed. So, the triplet  $[n_1 n_2 n_3]$  is comprised of smallest integers with same ~~relative~~ relative ratio.



For B, it is  $[111]$  and for C it is  $[022]$ . Thus, the direction is  $[311]$ . Note that, when we speak of a direction, we do not mean a particular straight line, rather a whole set of parallel straight lines. These parallel straight lines are equivalent by virtue of the translational symmetry.

When the unit cell has some rotational symmetry, then there may exist several non-parallel directions which are equivalent by virtue of symmetry. When this is the case, one may indicate collectively all the directions equivalent to the  $[n_1 n_2 n_3]$  direction by  $\langle n_1 n_2 n_3 \rangle$ . Thus, in a cubic system, the symbol  $\langle 100 \rangle$  indicates  $[100]$ ,  $[010]$ ,  $[001]$ ,  $[\bar{1}00]$ ,  $[\bar{0}\bar{1}0]$  and  $[\bar{0}0\bar{1}]$ , where the bar over the number indicates negative number. In the figure, the line AF, the direction is given by  $[100]$ . The opposite direction is  $[\bar{1}00]$ , however, equivalent  $[100]$ . The opposite direction is  $[\bar{1}00]$ , however, equivalent by the rotation along the line AF, the direction is given by  $[100]$ . The opposite direction is  $[\bar{1}00]$ , however, equivalent by the rotation symmetry. Similarly,  $\langle 111 \rangle$  describes the body diagonal directions of a cubic lattice.

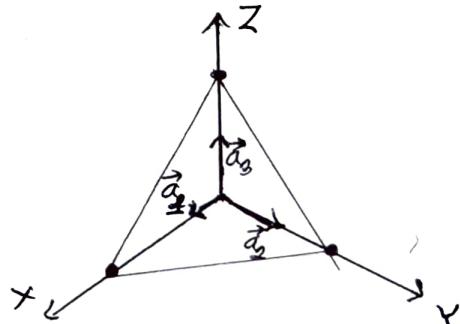
### Crystal planes and Miller indices

The orientation of a crystal plane is determined by three points in the plane, provided they are

not collinear. If each point lay on a different crystal axes, the plane can be specified by giving the coordinates of the points in terms of the lattice constants  $a_1, a_2$  and  $a_3$ . However, it turns out to be more useful for structure analysis to specify the orientation of a plane by the indices determined by the following rules -

1. Find the intercepts on the axes in terms of the lattice constants  $a_1, a_2$  and  $a_3$ . The axes may be those of a primitive or non primitive cell.
2. Take the reciprocal of these numbers and then reduce to three integers having the same ratio, usually the smallest integers. The result in the parentheses, (hkl) is called the index of the plane.

Consider the figure here. The plane intersects the axes, say at  $x, y$  and  $z$ . The basis vectors are  $\vec{a}_1, \vec{a}_2$  and  $\vec{a}_3$ . Usually,  $x$  is a fractional multiple of  $a_1$ ,  $y$  is a fractional multiple of  $a_2$  and so on. We form the fractional triplet,



$$\left( \frac{x}{a_1}, \frac{y}{a_2}, \frac{z}{a_3} \right)$$

You have to choose one and define all the planes according to that

We take the reciprocal of these ratios to find the triplet,

$$\left( \frac{a_1}{x}, \frac{a_2}{y}, \frac{a_3}{z} \right)$$

Then we will reduce the set to a smallest one by multiplying by a common factor. The resulting triplet  $(hkl)$  is the Miller index of the plane. In this example shown in the figure,  $x = 3a_1$ ,  $y = 2a_2$  and  $z = 2a_3$ .

So, the triplet is  $(3, 2, 2)$ . Inverting we get,

$$\left( \frac{1}{3}, \frac{1}{2}, \frac{1}{2} \right)$$

Multiplying by common denominator 6 we get the Miller index as ~~(2, 3, 3)~~  $(233)$ .

Note that, the Miller indices are so defined that all equivalent, parallel planes are represented by the same set of indices. Thus, the planes with intercepts  $a_1, a_2, a_3 ; 2a_1, 2a_2, 2a_3 ; -3a_1, -3a_2, -3a_3$  etc. are represented by the same set of Miller indices.

Therefore, a set of Miller indices specifies not just one plane, but an infinite amount of equivalent planes. We will see in x-ray diffraction from crystal structure, that this ~~way~~ of notation is nice to

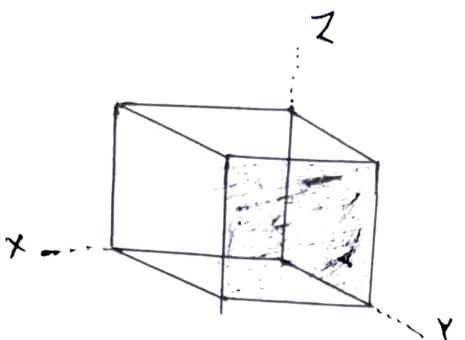
to study the diffraction.

The reason for inverting the intercepts to find the Miller indices is a bit subtle. We will see that the most concise, and mathematically convenient method for representing the lattice planes is using the so called reciprocal lattice. The connection will be discussed in the reciprocal lattice section.

Sometimes, when the unit cell has rotational symmetry, several nonparallel planes may be equivalent by virtue of this symmetry, and one writes the Miller indices to express all of them, in curly brackets,  $\{hkl\}$ . Thus,  $\{100\}$  in the cubic crystal system represents six planes -  $(100)$ ,  $(010)$ ,  $(001)$ ,  $(\bar{1}00)$ ,  $(0\bar{1}0)$  and  $(00\bar{1})$ . Here, the bar over the numbers represents negative numbers. So,  $(0,-1,0) = (0\bar{1}0)$  and so on.

A few examples of finding Miller indices

Let's see some examples where we find the Miller indices of various planes - of a cubic lattice.



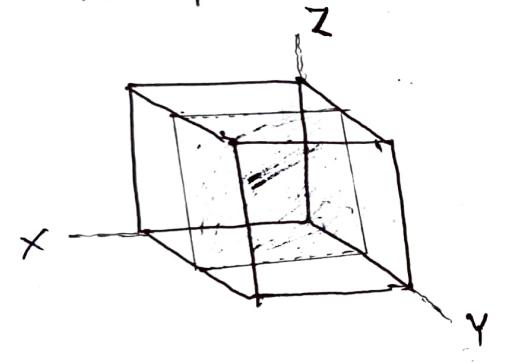
Intercept triplet:  $(\infty, 1, \infty)$

Reciprocal " :  $(0, 1, 0)$

Miller index:  $(010)$

For the opposite face,

~~intercept triplet:~~

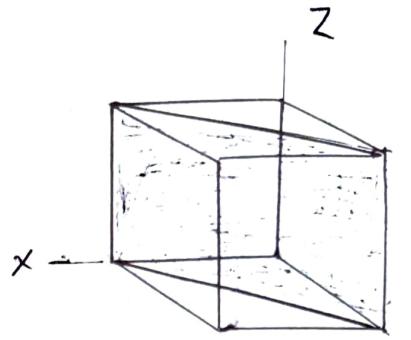


... :  $(\infty, 1, \infty)$

... :  $(0, 1, 0)$

... :  $(010)$

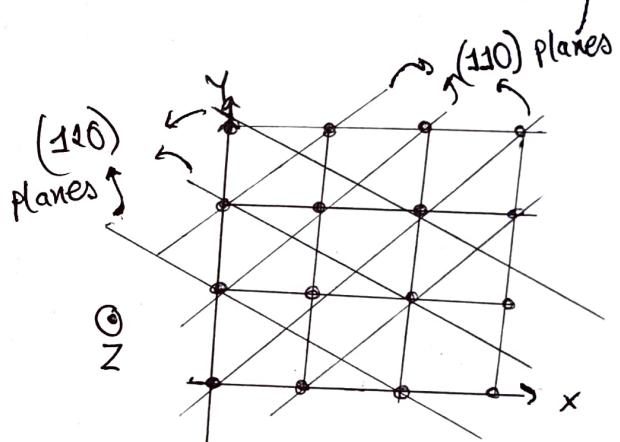
which must be true since  
it's parallel to the ~~one~~  
example (in the first)



Intercept triplet:  $(1, 1, \infty)$

Reciprocal " :  $(1, 1, 0)$

Miller index:  $(110) \nearrow$

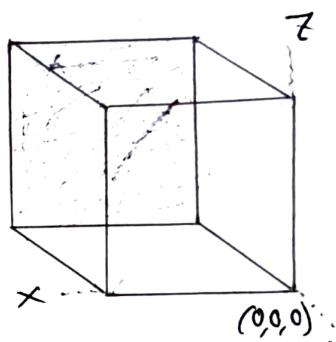
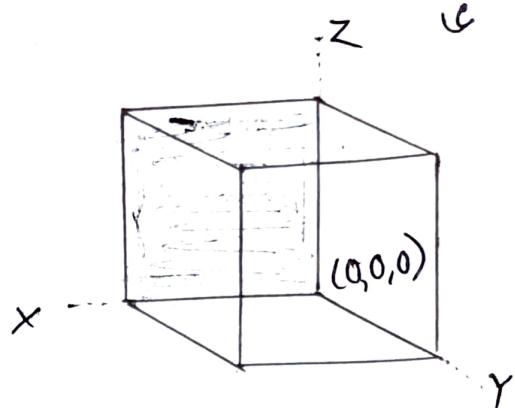


A set of parallel  
planes, having the  
same Miller indices

One particular problem that one can face is when  
the plane cuts the origin along a particular axis.  
For example, see the following example in the  
next page.

For the shaded plane, the intercepts are  $(1, 0, 1)$ , which is problematic, since you have to take the reciprocal of 0 here. In such a situation,

you need to shift the origin to the nearest lattice point of parallel face, like shown in the figure here. Then, the intercept triplet becomes  $(\infty, -1, \infty)$ . So, the reciprocal is  $(0, -1, 0)$  and so the Miller index is  $(0\bar{1}0)$ .



Spacing between planes with the same Miller indices

One often needs to know the interplanar distance between the planes with same Miller indices, specially in x-ray diffraction, as we will see later.

Say, the interplanar distance between the parallel planes with Miller indices  $(hkl)$  is given by  $d_{hkl}$ .

The actual formula will depend on the crystal structure, and we will confine ourselves to the

case ~~in~~ in which the axes are orthogonal.

Consider the plane as shown in the figure. We suppose a parallel plane to this passing through the origin.

Then, the interplanar distance  $d_{hkl}$  is basically the length of the normal line from the origin to the plane. Say, the normal line makes an angle of  $\alpha, \beta$  and  $\gamma$  with the  $X, Y$  and  $Z$ -axis. Then,

$$\cos \alpha = \frac{d_{hkl}}{x}, \cos \beta = \frac{d_{hkl}}{y} \text{ and } \cos \gamma = \frac{d_{hkl}}{z}$$

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

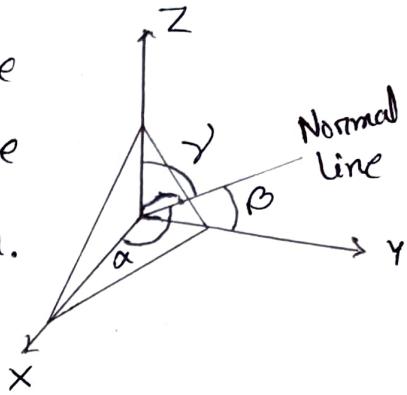
Also, the directional cosines satisfies the relation,

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

$$\Rightarrow \frac{d_{hkl}^2}{x^2} + \frac{d_{hkl}^2}{y^2} + \frac{d_{hkl}^2}{z^2} = 1$$

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

Now  $x, y, z$  are related to Miller indices.



$$h = n \frac{a_1}{x}, \quad k = n \frac{a_2}{y} \quad \text{and} \quad l = n \frac{a_3}{z}$$

where  $n$  is the common factor used to reduce the indices to the smallest integers possible.

$$\therefore d_{hkl} = \frac{n}{\left[ \frac{h^2}{a_1^2} + \frac{k^2}{a_2^2} + \frac{l^2}{a_3^2} \right]^{1/2}}$$

Thus, the interplanar distance of a cubic crystal ~~is~~ is,  $d_{hkl} = \frac{n}{\left[ \left(\frac{1}{a}\right)^2 + \left(\frac{1}{a}\right)^2 + \left(\frac{1}{a}\right)^2 \right]^{1/2}} = \frac{na}{\sqrt{3}}$ , where  $a$  is the lattice constant.