Symmetry and Structure in the Solid State
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Lecture – 30
Crystallographic Directions and Planes

So, we have been now you have enough knowledge gained now on Symmetry we have the basics of symmetry understood to the extent that we can now deal with crystals. So, in the last discussion we brought in the issue of a loaf of bread.

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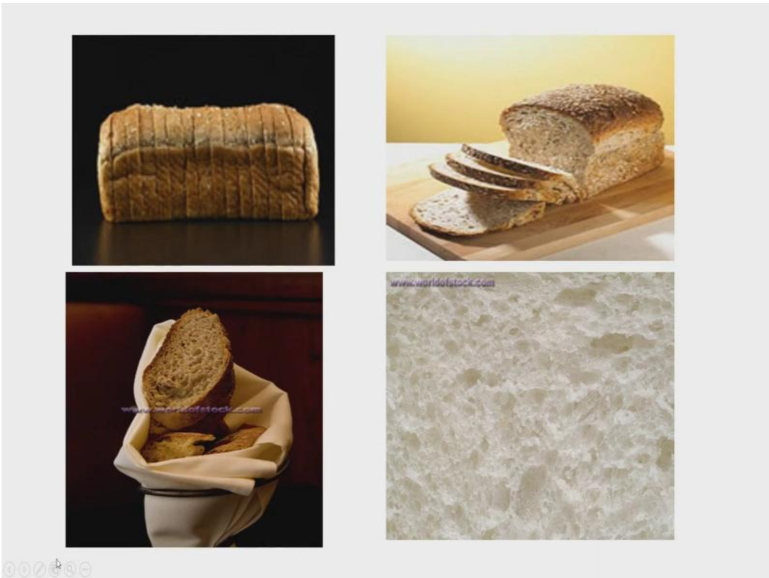

So, a loaf of bread now can be considered as a crystal and if we now look at the size of the unit cell. Let us say the loaf of bread is the size of a unit cell if we take this point or that point as the origin; when once the origin is fixed then this is the *a* direction let us say this is the *b* direction and the backside is the *c* direction.

So, it will say define the one these cell dimensions; from that we can calculate the volume of the unit cell by using the formula a . (b * c) and that will give us the volume of the unit cell. So, we also know that there are only 7 types of unit cells we can think of and those unit cells will give the dimensions according to the definitions of *a b c* and the interaxial angles between them.

Having noticed that we now also in fact, can identify the various possible planes through this unit cell volume. So, the here is the volume of the unit cell and then we now slice the unit cells into a number of pieces like we slice the piece of bread. And suppose I take the midpoint of a as a and then cut it and take that slice out that very thin slice out that slice will be equal to ½ the unit distance along *a*. And of course, if we consider this particular point which I am showing now that will be 0 0 with respect to *b* and *c*.

So, this is referred to as the crystallographic direction we will in fact, describe these crystallographic directions in detail in a couple of minutes. So, the direction through the unit cell is referred to as the crystallographic directions. So, if you go along this direction it is 1 along the *a* direction. So, this particular point will be 1 0 0; on this direction of *a* will define 1 unit along *a*.

And if we now consider the 0 0 the intersection associated with *b* and *c* and if we take that slice out that slice will be 1 0 0 and the slice which is at ½ point is 2 0 0 at one third is 3 0 0 and so on. So, these numbers which we give 1 2 3 etc.., they refer to the so called *hkl* values and this we will define in a few minutes as the Miller indices. And these *hkl* values define they play any given plane in a crystal. So, if we have these *hkl* values given to you; you have to identify them with respect to your plane.

So, how do we identify the crystallographic directions then; what are the identities we can give for a direction in a crystal?

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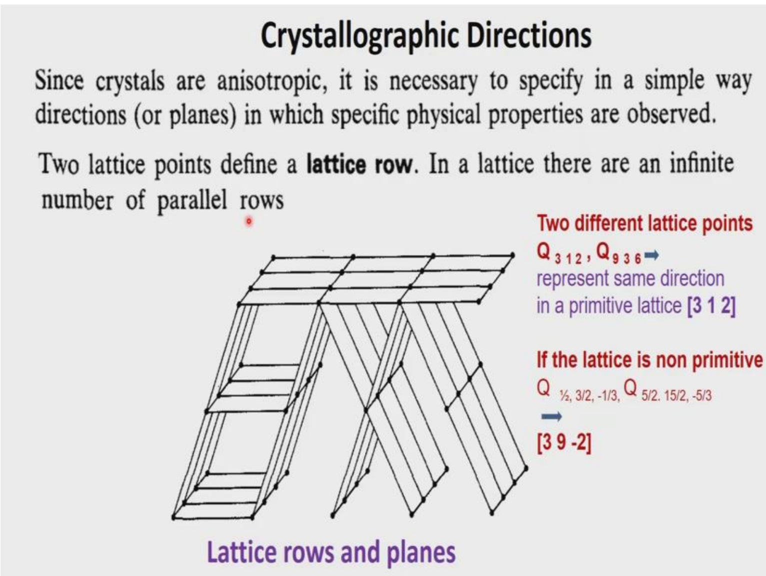

So, that can be seen from this illustration down here. So, we have because you see the single crystals which we grow are anisotropic. So, it is necessary to specify the simple way in which we can define directions or eventually planes in which we have to observe the physical property.

Suppose let us say with the property of a given crystal it shows ferroelectricity or for that matter it shows some specific physical property in a given direction. We have to specify the direction in the crystal; the reason is that in the other directions the same property may not be expected may not be present.

So, this is a property of the material; so, if we are looking for the property of the material into which we have of which we have grown a single crystal then the single crystal will have to be specified with respect to the direction or the plane about which these physical properties are measured.

For example, it could be a certain value of the dielectric constant which is now measured along a particular direction. So, when we have single crystals therefore, we identify the directions put those directions in the device which will measure that property and we can measure that property in that given direction. So, these therefore, the definition of a crystallographic direction and plane become extremely important.

These points are or probably not very well explained in any textbook, but in these discussions we will go specifically with respect to the understanding of the crystallographic directions and planes; with the view that we are going to measure physical properties later on.

For example, if you are measuring the elastic constants of a given crystal the elastic constant direction has to be specified. So, we will have a just like anisotropy in the single crystal we will also have anisotropy in the elastic properties; these as anisotropy can be expressed in terms of a matrix and those matrix values can be calculated.

So, to make it very simple we will now take any 2 lattice points let us take this diagram here any 2 lattice points and then continuation in that particular direction defines what is known as a lattice row. So, for example, this is a lattice row that is a lattice row and that is a lattice row. So, a row of lattice points is referred to as a lattice row and this could be along *a* direction it could be along b direction it could be along *c* direction; it could be along any direction inside the unit cell and that needs to be particularly specified.

So, as you see that in a lattice there are in infinite number of parallel planes the illustration here shows a few of them; so, you can draw any number of them. So, if we take two different lattice points just to make points clear if we take two different points $Q_{3\ 1\ 2}$ for example, Q represents the vector in the direction of 3 1 2 and that represents a given direction. So, if you take the Q as the value associated with the direction 3 1 2; this is a measure the vector distance is a measure of where the 3 1 2 comes with respect to an origin; obviously, we need a definition of an origin.

Suppose let us say I define this as the origin and take this as 1 2 3 that will be a 3 position and then I have a one in the direction perpendicular to that; so, I can take this and that as 3 1. Now if I want to represent a direction which is perpendicular to that I can take this direction. So, for example, if the point here can be represented in terms of the origin here as 1 along this direction, 2 along that direction and 0 along the third direction. So, these therefore, now defines a direction way from here to here one can define a Q vector. A Q vector therefore, is a direction dependent vector and that can in case of 3 1 2 can be represented within this diagram.

Suppose we take something like $Q_{9\ 3\ 6}$ which is far away in the unit cell; now we would like to find out whether 3 1 2 and 9 3 6 represent the same direction. In fact, they do represent the same direction if it is a primitive lattice and that is because of the fact that 3 1 2 and 9 3 6 have a common factor between them. So, you can take the common factors that is 3 times 3 is 9 1 times 3 is 3 and 2 times 3 is 6.

So, once again 3 1 2 and 9 3 6 they represent the same direction. So, when we say the in bracket [3 1 2]; it comprises of all possible directions in that orientation of 3 1 2. 3 1 2 is a specified direction and we have to therefore, represent all the lattice points in that direction. So, if we now put this square bracket it represents all possible directions in 3 1 2; if we just say 3 1 2, that will refer to the with within the bracket as we have shown here the then it represents the direction 3 1 2 and all the family members which are factorizable under 3 1 2 belong to this direction.

The points are different, but the direction is the same; so, when we say 3 1 2 that specifies the direction. So, the specification of the direction is by crystallographic nomenclature done by the brackets; the square brackets [ ]. You might look into a situation when it is a non primitive lattice. A non primitive lattice is one in which we do we have centering for example, we have a *C* centered lattice, we have a *F* centered lattice, we have *I* centered lattice and so on in which case the lattice points may occur at 0 0 0 and also at ½ ½ ½ which is a fraction.

So, if the lattice points are fractional like is shown here where direction Q which is 1/2 3/2 -1/3. And then there is a direction which is a Q which is 5/2, 15/2,-5/3; both of these represent a single direction in crystallographic direction and that crystallographic directions happens to be [3 9 -2]. How do we get [3 9 -2] with these two? What we have to do is we have to take the LCM of the lower numbers 2, 3 and 3; we take the lowest common multiple and then we represent them then we represent the direction.

So, we see here for example, one ½ ; one ½ times this is 6. So, 1 by it; so if we multiply this by 3 ok, if we multiply this quantity by 3 then the least common multiple is 6; so, you get what? You get ½ . So, 3 by 6 is ½ and 9 by 2 and in this particular case it is 9 by 6. So, it will be 3 by 2 and so on. So, the same thing happens to the logic here you have to take the LCM of these three numbers and these three numbers and these three numbers in the denominator or common and therefore, we the representation of the direction is [3 9 -2].

So, we get to represent both the direct lattice points in the primitive lattice as well as in the non primitive lattices by this kind of direction identification. A better way to look at it is to take several fractions and then see what direction it represents by taking the least squares LCM of these numbers at the as the lower part of the fraction the denominator of the fraction. And then calculating the corresponding planes which will represent the top part; so, which is the numerator of that. So, effectively what we do is we once we take the LCM we cancel out that number and whatever number remains in the numerator is represented here.

So, if you do that operation on these two cases you will get [3 9 -2]. So, this brings us to an idea of how we represent crystallographic directions in a unit cell. So, now, it is possible therefore whether it is a primitive cell or a non primitive cell; it is possible to identify directions in terms of 3 numbers and 3 integers rather. And these 3 integers could be both positive as well as negative depending upon where you define your origin.

So, the origin definition becomes crucial and one once we have 0 0 0 defined then all the directions in the crystallographic unit cell can be identified. So, there are numerable number of such things infinite number of such possibilities and all these possibilities are accounted for. And also many of the lines many of the lattice points will form which will lie on the direction of this crystallographic direction which we have defined all those lattice points will also belong to the same direction. So, there may be a large number of lattice points in a given direction there will be less number of lattice points in a given direction depending upon the value of the unit cell in those directions.

So, the unit cell decides what should be the total number of crystallographic directions we can have in a unit cell. Of course, the unit cell will itself have the possibility of 7 different types of lattices. So, the lattices both primitive as well as the centered ones or the non primitive lattices can be covered under the definition of crystallographic directions.

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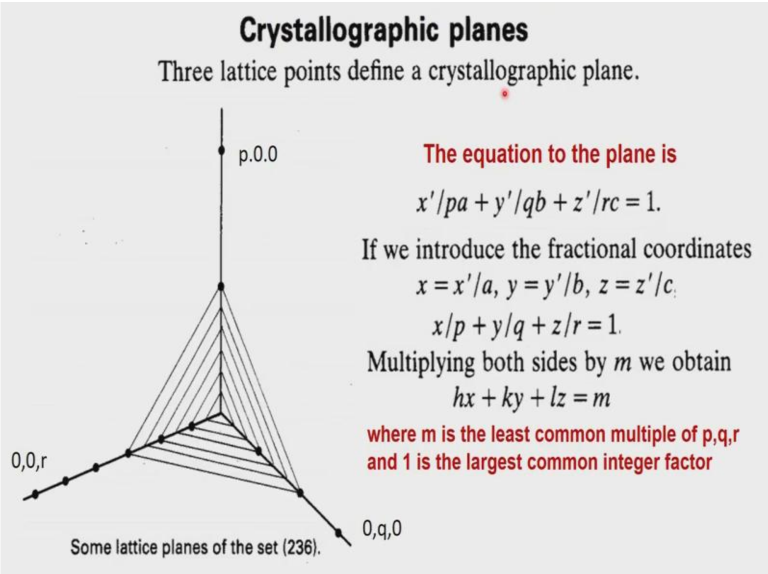

So, having learnt what crystallographic directions are we will now go to the crystallographic planes. In case of a crystallographic planes we need 3 lattice points the diagram below is shown here it represents the 2 3 6 that is because I have shown two along this direction 2 units and then you see the lattice points two are along these direction and here it is 1 2 3 4 5 6 along the vector r along the vector p it is 2 and along the vector q it is 1 2 and 3.

So, this now let say tells us that if we join these 3 points p 0 0, 0 0 r and 0 q 0 from the origin which is at 0 0 0 this now represents the plane 2 3 6; 2 units along the x axis 3 units along the y axis and 6 units along the z axis and that represents the plane 2 3 6. If we write 2 3 6 in brackets [2 3 6] it represents all planes which are parallel to this plane and depending upon whether it is a non primitive lattice or a primitive lattice; we can have a number of lattice planes.

And these are all parallel planes as we have seen drawn here this is one plane this is another plane which is passing through this lattice then there is a plane passing through that lattice point and so on. And eventually we have a lattice point which passes through these 3 this will be actually the family 2 3 6; even though we now see it is 1; 1 2 3 along these direction and 1 2 along that direction.

So, the lattice planes belonging to 2 3 6 can be represented in this fashion. All the lattices lattice planes which come within the 2 3 6 direction will be less than the 2 3 6 value of the unit cell. Now the we have to develop an equation to this plane; so, equation to any plane is the value of x in that direction and the total length a.

So, suppose we have a unit cell a b c then the equation to the plane is along a we can have a x'/a fraction which can represent our. For example, if we take this as p then the fraction is x'/ pa and x is the direction of the unit cell and if the value of the unit cell is a; we restrict the direction to stop at the point a because we it repeats again because of the periodicity.

Because of the periodicity nature we have therefore, the unit cell a unit cell b unit cell c representing the unit the entire unit cell unit directions. And then x'/p y'/q and z'/r represents the fractional units along those 2 3 directions. And therefore, this will be the equation to the plane and that we equate equal to 1. If we now introduce the fractional coordinates and that is why time and again we have mentioned even in our earlier discussions; that when we refer to a position x y z it represents the fractional coordinates associated with the system. It is because now we define the fractional coordinate x as x'/a y'/b and z'/c.

So, therefore, you can write the equation to the plane as $x/p + y/q + z/r = 1$. So, this is the equation to the plane; so, any plane in the crystallographic unit cell can be defined by this particular fashion $x/p + y/q + z/r = 1$. Now we multiply both sides by a quantity called "m" which is an integer; this is because of the fact that we want to represent the entire set of planes in all these intersections. And in order to do that we have to now take the common least common multiple of *p q r*.

So, we take the least common multiple LCM of *p q r* and that represents all possible values of m which will now be equating to this plane; that represents the family of planes. This is a single plane which is 2 3 6 in these example we have given here and the $hx + ky + lz = $ m; where m is an integer represents all these planes that are possible inside this representation of the 3 lattice intersection points which hold a plane.

So, *p q r* now, therefore, define the plane 2 3 6. So, we have seen therefore, the way in which the crystallographic directions and the crystallographic planes can be mathematically calculated. But we want to make it as simple as possible in our discussions we have kept it at a very simple level.

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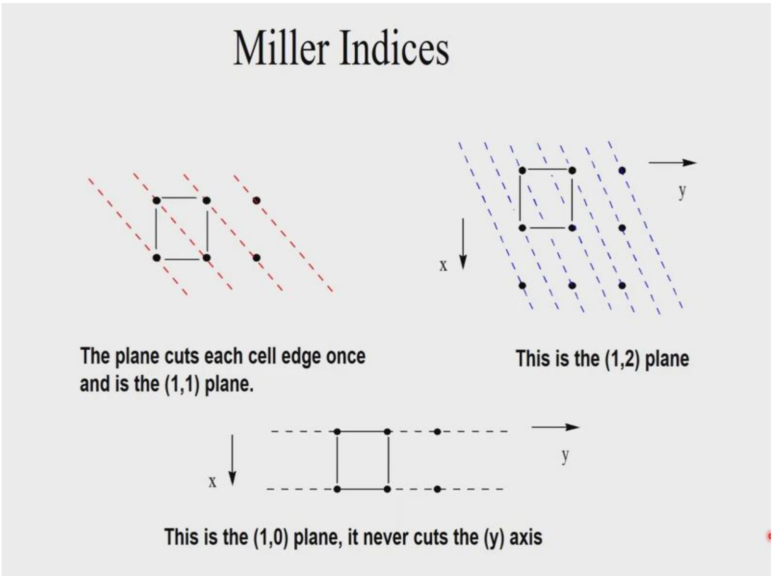

And so we will look at it this way. So, suppose you take in you know we always want it in 2 dimensions it is easy to understand in 2 dimensions.

So, the we now have to see that the third direction is coming towards you. So, it is a 3 dimensional unit cell and in this unit cell the lattice points; let us say this is the *a* direction and this is the *b* direction these are the lattice points ok; these are the lattice points this is *a* and that is *b, c* is coming out towards us.

Now if we want to represent the so called one unit along *a* and one unit along *c*; now these lines which we have we have drawn now represent the entire family of 1 1. The family that is associated with 1 along *a*, suppose this is the origin this is the one value of *a* and that is the one value of *b*.

So, the entire family of 1 1 is illustrated by this set of parallel planes of course, we at this particular way position consider the line here and the *c* is coming perpendicular to that and that is taken as 0 in these example. So, if we take this 2 dimensional case we have the 1 1 and I still call it a plane because we have the *c* direction perpendicular to that; so, this is the 1 1 plane in 2 dimensions one along this one along that. Suppose we look at this picture in this picture you see they even though there are points which are now corresponding to lattice *a* and lattice *b*; you see that there is an additional point which comes ½ way along a and ½ way along b and these now all are also parallel lines.

So, when you consider these parallel lines; you see that now we have to represent this as the as far as *b* is concerned we have divided into ½ and ½ , *a* is still the same as before the *b* direction which has been cut into ½ and therefore, this becomes 1 2. In that discussion in the same way we can now define the; so, called 1 0 plane because if you just take the *x* direction and this is the value of one and then *y* will be like this. So, the 1 0 plane will be running parallel to the *y* axis.

So, all the planes which are running parallel to the *y* axis will belong to 1 0 plane. So, *y* is the direction *y* is the direction of the unit cell and the planes are now parallel to that in the sense that this 1 0 plane; the family of 1 0 plane 1 0, 2 0, 3 0, 4 0, 5 0 whatever be the number all of them will be parallel to *y* axis. In this case all of them will be 1 2 planes of entire family of 1 2 plane; that means, 2 4 and 3 6 all these will be also belonging to this family of planes. So, the family of planes therefore, are represented in brackets; let us see how we can generalize it a little more.

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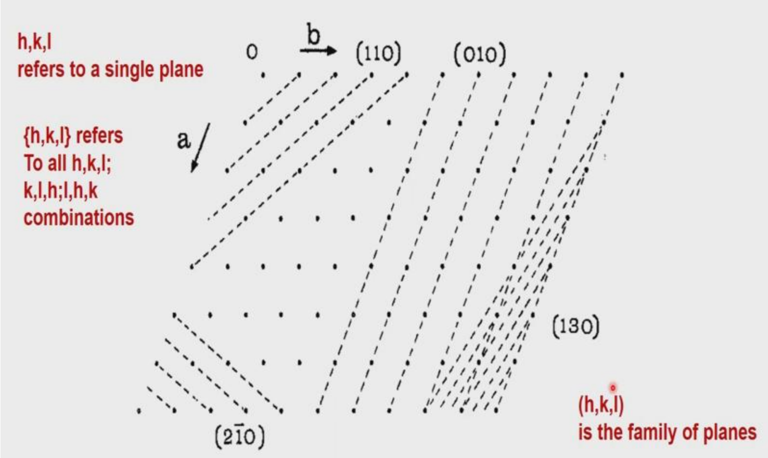

Fig. 1.6. Miller indices for some crystallographic planes parallel to Z (Z is supposed to be normal to the page).

We can generalize it a little more by looking at this diagram. Now this diagram tells us that we have a lattice this is the 0 point and these are the lattice points along the *a* direction and these are the lattice points along the *b* direction and these are the lattice points which define our unit cell.

And so, this now if you consider this point this point this point this point these 4 now define the values associated with in 1 units of lattices. And let us say this is the primitive lattice; if we consider that as a primitive lattice then we have this family of planes which is one along *a* and one along *b*; you see this is the origin ok. So, you take one along *a* and one along *b* you get this plane.

Now, you can draw a parallel plane now this parallel plane cuts at 1 and 2 along this direction 1 and 2 along that direction; the value of *c* is equal to 0 because we are now taking the projection *a b* and so, this is 1 1 0. So, the family of planes is now represented as 1 1 0. So, the when whenever we write a bracket like this it represents the family of planes. If we do not write any bracket and just write 1 1 0 by crystallographic nomenclature 1 1 0 refers only to that plane.

So, suppose there you are trying to say where the atom is sitting in which plane a given atom is sitting; this atom may be sitting at 1 1 0 then you do not write the brackets. Because if an atom is sitting at 1 1 0 it does not mean it will sit at all the parallel planes understand.

So, if there is an atom sitting at let us say 2 2 0 and then let us say there is a whole 5 or 6 atom sitting in 2 2 0 ok; then it is not necessary that any atom need to sit at 1 1 0, but these are all parallel planes. So, since they are all parallel planes the family of planes is represented in bracket and when we look at the scattering in a few minutes from now; you will see that the scattering is dominated by these planes.

So, let me now bring that discussion now itself, but we will make it more clear as we go along. What we do is we have a unit cell and that particular unit cell is like this a loaf of bread; now this particular unit cell can be cut into a large number of planes; we can have defined crystallographic directions we can have crystallographic planes and so on. And so when we now send a probe which could be a electromagnetic radiation, it will go through this loaf of bread and it will pass through all these planes all these directions; all these planes.

Now, suppose we now populate these planes with atoms; let us say as we discussed in the last part of our previous discussion. Suppose this is a special bread and you have additives in this you may have cashews added, you may have badam added and so on. So, we do not know where these additives are sitting inside the loaf of bread it is not visible; so, but when we slice this and take a take a plane out of this slice, let us say we take 2 0 0 in that particular slice we may find a piece of badam and a piece of the cashew.

So, a same logic can be applied to atoms inside the unit cell; the atoms and the molecules are whatever which exists inside the unit cell are now distributed inside the unit cell among all these planes. But what we do in a diffraction experiment which we will do soon is to now shine some radiation electromagnetic radiation. The electromagnetic radiation will go through the crystal it will go through the crystal it is like entering a rarer to a denser medium and then it will emerge to a rarer medium. So, there will be reflection, refraction all kinds of possibilities that can occur with waves; same thing will happen, but then if these planes are now populated with let us say these additives like for example, atoms of different sizes and different electron densities and so on.

Electromagnetic waves are made up of electric waves the electric field is associated with an incoming electromagnetic wave. These electromagnetic wave even the ordinary light is an electromagnetic wave as you all know; so it has an electric component. So, when it looks at an atom let us say that particular atom will have its own characteristics; particularly it has an electron density around the central nucleus.

And that electron density responds to the incoming scattered radiation incoming radiation and then it scatters the radiation. It finds it is something like you know you are moving in a crowded town centre and you are going in a straight line, but then a group of 10 people come in front of you will have to either go away from them or shoulder them and go through.

So, that is exactly what happens to the incoming radiation it finds the atoms and therefore, electron density in its path and when it finds that it has to scatter it has to move in a different direction and that is exactly what we will happen. And therefore, we have to now see what is the consequence of such experiments which we are going to perform on the crystal.

So, to continue our discussion at the moment we have defined the crystallographic directions, we have defined the crystallographic planes we have to completely now finalize how to define the crystallographic planes. For example, here I had shown you the 1 1 0 set of planes; here the this shows the 0 1 0 set of planes that is the all those planes which are parallel to the *x* axis ok; all those planes which are parallel to the *x* axis and of course, we are taking 2 dimensional plane here. So, it is *c* is automatically set to 0.

So, 0 1 0, 0 1 0 represents this and suppose I now want to represent 1 3 0 you see that the 1 3 0; that means,1 along the *a* direction and 3 units along the *b* direction. So, this has to move up here and this is 1 2 3 and those are now the parallel set of 1 3 0. And similarly 2 -1 0 is shown in order to for you to understand the way in which the planes develop with respect to the crystallographic unit cell *a* and *b* with an origin defined.

So, you have the family 1 0 0 sorry 1 1 0, 0 1 0, 1 3 0, 2 -1 0 and when we have put these normal brackets ( ) around it represents all the planes from 1 equals 1 to n and 1 to n and in this case one goes from 1 to n.

Here 2 goes from the value of 2 to 2 times the next value that is again 2. So, it will be 4 -2 0, 6 -3 0 and so on; so those are the parallel. So, all parallel planes get represented as families; if we just want to refer to one particular plane as we discussed suppose there is one atom only at this particular plane; then we say that the atom is associated with a *hkl* plane. That *hkl* now you see has no brackets around it, so we are now identifying that particular plane *hkl* about which the atom position is located.

So, if atom is located here we say that the atom is located with respect to the plane 1 0 0; it is always possible to locate atoms anywhere in the unit cell, it is not necessary that they should be associated with the lattice planes. But when we do the scattering experiment as I already defined the scattering experiment is happening with respect to the planes. So, there may be an atom associated with the plane, there may not be an atom associated with the plane, but the when light comes and falls on that light will get scattered and that scattering is independent of whether it has an atom or not.

So, if there is no atom it will pass through the crystal and there is no scattering occurring. If there is an atom as I said there will be some disturbance and therefore, scattering occurs. But if there are atoms which are situated between these 2; suppose there is an atom here this atom now contributes to all the parallel planes, it not only contributes to the parallel planes it also contributes to the planes which are in other directions as well. So, that is something which we will evaluate in a couple of classes from now; what is the contribution of the atom to a given plane.

So, to cut the long story short here is a gist of what I would like to say in the last half an hour's discussion and this is very very crucial. What we now want to do is to examine the inside of the unit cell we have now understood that there is symmetry, we have understood all possible symmetries that can occur inside crystals, 7 crystal systems 32 point groups 230 space groups; we now thoroughly know where the equivalent points come in a given space group what is the special position and so on.

Now, these are all the possibilities that can occur inside a crystal; we have understood also the way in which the lattice develops itself in 3 dimensions to define the structure to define the crystal. So, having got that basic information and having understood all rules of symmetry; we now consider situations where atoms and molecules can get inside this crystal, but the way the atoms and molecules are getting inside this crystal is like the additives getting added inside the bread loaf.

But what we are going to measure in X ray diffraction techniques which we are going to discuss in a few minutes from now is the fact that it is coming from the planes. So, whatever scattering is occurring; the incoming radiation now will see these planes and these planes now will scatter the incoming radiation. So, whether a particular plane which we identify here is having an atom or not; the atoms which are present inside the unit cell will contribute to that.

So, we have to see a what in what way they contribute to that and in what way we get to the scattering information from that particular plane. Obviously, if we get all the information from the scattering planes of this kind; in principle we should be able to guess where these little pieces or in fact, the pieces of whatever additives we have added in this particular example what are the atoms and where they are sitting inside the unit cell.

So, we can identify the atomic positions we therefore, can identify the bonding associated with the atom positions and hence the structure that is associated with the atom. So, the logic therefore, is that when we do the crystallographic measurement; now which we are going to do on a unit cell which about which all the rules and regulations about which have been framed by us already. So, we now know the grammar of the situation, we can now construct a novel.

The construction of the novel now goes the fact that we have now to determine what is there inside the unit cell; what is there in the unit cell or the atoms and the molecules and so on which consists of nuclei and the electron density around it so happens that when X rays fall on a given atom we will see in a few minutes. When X rays fall on a given atom it is the electrons that scattered; X rays normally do not approach the nuclei they do not have the power enough to approach the nuclei. And at the same time the X rays which are used are about 1 Å in diameter in sorry in wave length and the atom has a diameter in the range of angstroms and therefore, the electron density around the atoms or in the range of angstroms.

So, essentially the electron density it is the electrons which scatter X rays; we should never forget it when we do our X ray analysis. Because whenever you probe through X rays you will see the electron density; whenever you probe through just to information sake whenever you probe through neutrons, you get the positions of the nuclei. And whenever do you do electron diffraction again you will get the electronic information. So, these are issues which we will discuss more and more in order to understand where the atoms are sitting.

So, the take home from this slide is these are the definitions of the planes, different kinds of planes, we have family of planes, individual planes are represented like this. And there is one more representation which I must mention here is the representation of *hkl* in flower brackets { }. When you see them in flower brackets it refers to all the *h, k, l; k, l, h; l, k, h* and so on. So, this is entirely dependent upon how symmetry dominates the *hkl* values.

And in other words how symmetry controls the orientation of the planes and this kind of restrictions come in only higher symmetries crystal systems. Cubic systems have this that for example, in a cubic system since a = b = c, $\alpha = \beta = \gamma$ are 90^{o}, 100, 010 and 001; these are all one and the same because we cannot distinguish between *a b* and *c*.

So, when we now represent the *hkl* associated with it; all these get represented not just 100, -100, 010, 0 -10, 001 and 00 -1. So, it is degenerate to that extent because *a* = *b* = c and so, such planes are represented in flower brackets. So, when you write in flower bracket and say 100; it represents all the 6, I mentioned in the case of a cubic system.

So, these are the nomenclatures. So, *hkl* alone and represents one plane; *hkl* in brackets ( ) represent now the family of planes and *hkl* in flower brackets { } represent all combinations of this depending upon the symmetry conditions which we impose. Now once again to generally remind you that if I have a square bracket and say [110]; it represents a crystallographic direction. Suppose I have a square bracket and say [111]; it is the diagonal of the particular unit cell whatever is the unit cell.

So, the crystallographic direction is therefore, different from the crystallographic plane and that is that is what we learned in the last half an hour or so. And so this is something which is very crucial for us to remember and when we lead read literature; in literature people normally refer to these without any introduction to what they are writing about and therefore, it is important to know these nomenclatures.