Material Science
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Lecture No 4
Crystal Geometry

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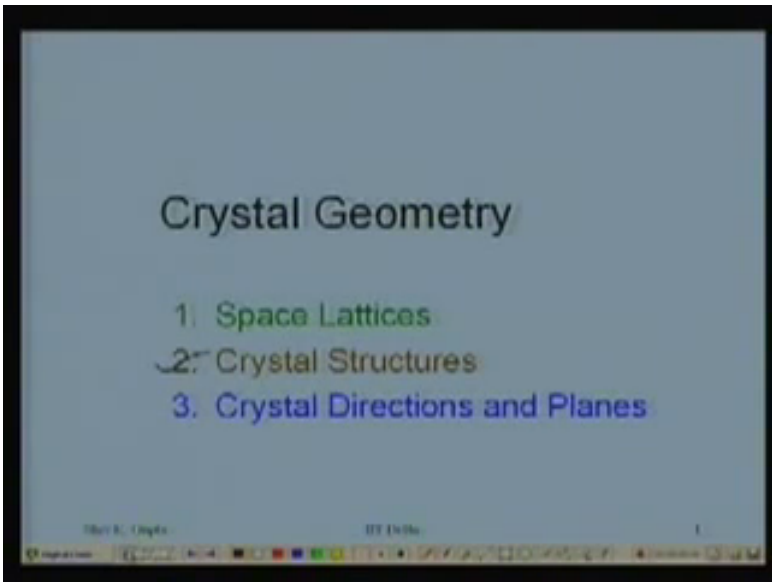

Friends in the last class we talked about the space lattice in the crystal geometry and today we shall start with the crystal structures and then move on to the crystal directions and planes in three-dimensional crystals.

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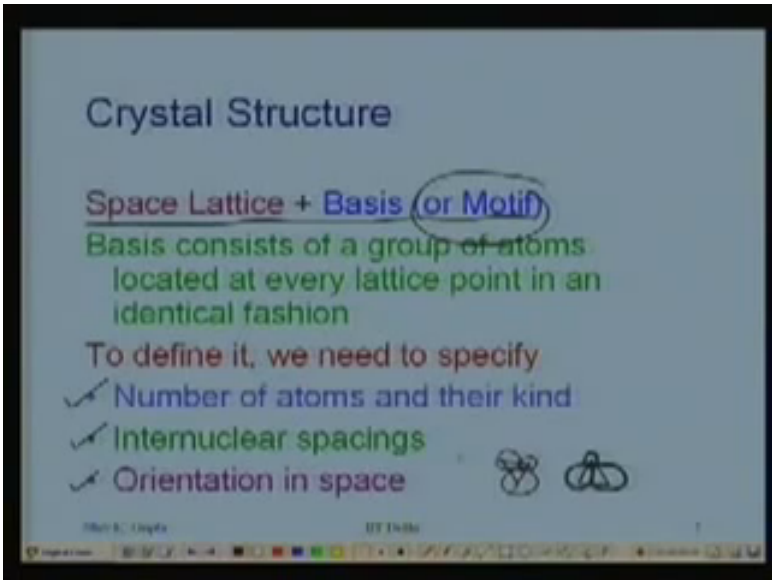

We define the space, Bravais space lattice is only 14 but as we know there are thousands of crystals already known to us and they are listed in the literature, so with the help of this 14 space lattices we have to understand these various substructures. To define the crystal structure as space lattice and basis, as I said earlier before I started defining these space lattice, I said crystal has a periodically repeating arrangement of atoms or group of atoms, so to understand that we 1st saw the arrangement of points, geometrical points in three-dimensional space having seen that now uhh so we shall associate with each point which was a geometrical point no physical entity, a group of atoms or molecules what I am calling Motif or the basis of crystal, okay.

Now this basis is the simplest if I have only one atom in it I do not have to define anything except saying it is a copper atom or it is an iron atom or it is a zinc atom, so I have to just specify that the kind and the number is only one becomes very easy but once the uhh moment I have 2, 3 or more number of atoms in the group which is sitting on every lattice point or associated with every lattice point I need to define number of things, I need to define number of atoms and their kind, I need to define the spacing between those atoms that is internuclear spacing how the group is arranged?

Then how this group is oriented in three-dimensional space? Let us say what I mean the orientation would become clear to you after I show you some pictures. I have this group which forms lattices joining the centres a figure like this or a triangle. If this triangle arranged like this or this triangle is arranged like this in space that is what I mean by orientation. That is what you have to see, so we have to understand the orientation in space that we shall see with the help of simple examples.

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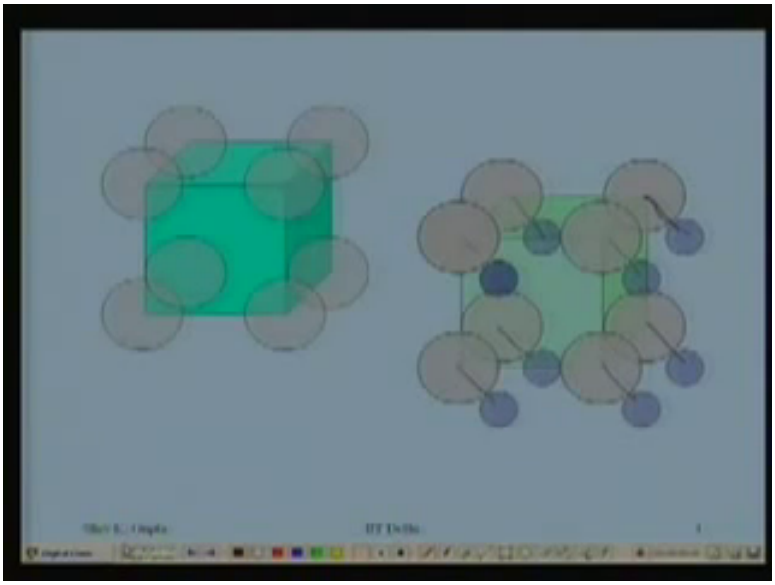

Here I show you a very simple example of a simple cubic space lattice, lattice points are at the 8 corners of the cube and I associate one atom on every lattice point and I get crystal unit cell like this see. If I associate with the same space lattice set of 2 atoms or group of 2 atoms the motif contains 2, one is this atom the other one this, this is associated with each lattice point in the same orientation and the spacing between the 2 atoms centre to centre distance is also the same. Centre to centre distance between them is same everywhere and the line joining this centre to centre if you see the orientation three-dimensional space is the same.

As a matter of fact it is possible for me to join the centre of smallest spears make another unit cell which is identical to the already down unit cell. So I need to define when we have 2 this is atom of one kind this is the atom of the 2nd kind I have to name them it could be a copper atom this could be a zinc atom, okay. Then I have defined the distance between them well for that I shall explain to you that these atoms while trying to understand the crystal structure we are going to assume that they are hard spears.

Though we know from the knowledge of chemistry that there is a nucleus around which their number of electronic orbits and this electronic orbits are not solids in the sense they are compressible electron clouds they can be extended too but we shall assume these to be hard spears for understanding the crystal structure, the periodic arrangement and whenever it comes we will try to know that just it is not a hard spear. So this is the internuclear spacing is defined and then orientation in space is got to be defined, alright. I shall show you another arrangement where the 2 atoms of there associated with every lattice points but the orientation in space is different, internuclear spacing is different, crystal we get is different.

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See the same thing in here the same unit cell shown here, now the 2 atoms arrange internuclear spacing is half the body diagonal of the cube and the orientation is along the body diagonal of the cube, this crystal looks very different from the previous one though there are only 2 atoms associated with every lattice point. Here you will ask me where is the 2nd atom associated for this it has to go to the next unit cell from there I have to go to another unit cell, each corner I have to go to another unit cell to find that and this form a different crystal altogether though I still have the 2 atoms forming the motif but the motif is different it is oriented in space differently I get a different crystal like this one example could be that of CCM chloride, this could be the CCM ion sitting here at the body center and these are the chloride ion sitting, I got a CCM chloride crystal like this, so we see that motif or the basis the group of atoms as to be associated with every lattice point I get a crystal, right?

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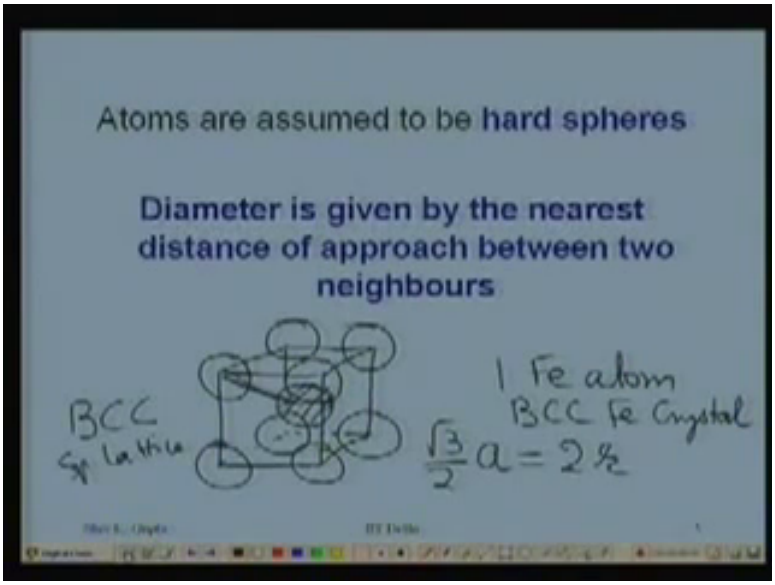

Well as I already said the simplest of the arrangement could be in the motif only one atom and 2, 3, 4 they are going to form a little more difficult motif but there is one element from group 7 which is manganese, it shows number of allotropic form one of them is alpha manganese at room temperature this space lattice is body centric cubic and there are 29 atoms in the motif, 29 not 1, 2 or 3. The 2nd form of the manganese, the body centric cubic uhh sorry the beta manganese form the space lattices is simple cubic and there are 20 atoms sitting on the motif but if I go to some of the polymeric crystals or maybe protein crystals there could be 10,000 20,000 atoms in the motif or more complex structures, we shall restrict ourselves to common materials which we are using and they have one or 2 atoms in the basis usually and the motif is simple will be able to understand that.

Now talking about the hard spears we define the diameter as the distance of nearest approach, so for example I just showed you one unit cell let me show you another one. Here the atoms, this is let us say a BCC space lattice and I have this motif as 1 iron atom it is sitting 1 iron atom is sitting at each lattice point which are at the 8 corners and one body center there, right? So this becomes BCC iron crystal. The distance of nearest approach is not atom from one corner to another corner but one atom from the corner to the body center that is the shortest distance between the 2 iron atoms and this distance is half the body diagonal.

The lattice parameter of the unit cell is a under root 3 by 2 of a, this is equal to the diameter or the twice the radius of iron atom that is what I mean when I consider them to be hard spears, however like the example I showed for CCM chloride this atom is different from the other one then the radius of his plus the radius of that channel becomes half the body

diagonal, again that is the meaning of the hard spears, I considered them to be hard spears, okay so that you understand the crystal structures well.

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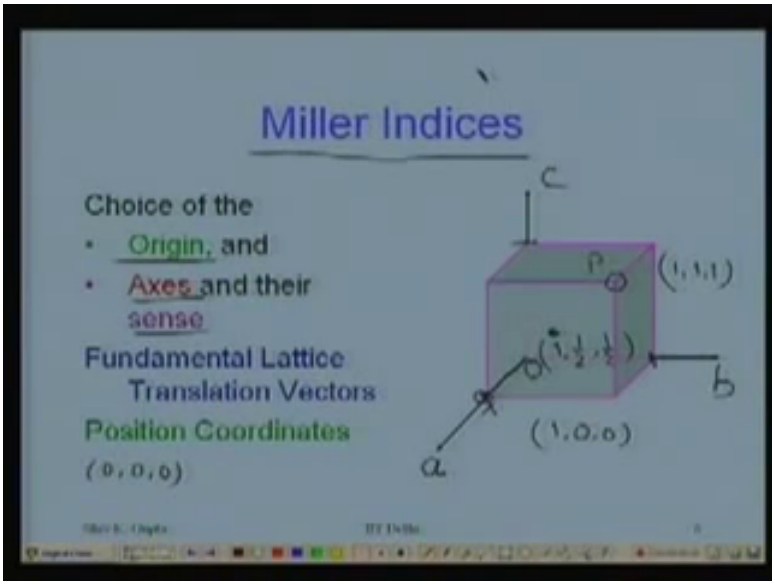

Alright with this knowledge of the crystal structures and the arrangement of points in three-dimensional space, now I am interested in looking at the directions after the points in geometry you are always taught the lines but instead of lines here I am interested in direction. Direction is a line right but it has an orientation which we always show with the help of an arrow it will show the sense of direction if I show the arrow, okay. So we give the names of these directions in crystal and these names are called Miller Indices.

We give names to all a little directions in the same orientation or same sense one name, all parallel directions which may be there in a crystal pointing in one particular direction they are given one name. If they are pointing in the opposite direction name would be opposite, what is that opposite? We shall see that, for this how we go about is the 1st of all choose the origin and the choice of the origin is arbitrary, normally we put the origin at the lattice point and if there is a unit cell which could have one lattice point per unit cell, 2 lattice points or 4 lattice points depending on where the lattice point is I can choose my original.

This choice is arbitrary and left to the user, okay and you can…same crystal understanding one problem and the other problem you can shift your origin or trying to know one direction and the other direction you can shift the origin of the axis and their sense once you choose you will not change otherwise you will lose the relationship between various directions, okay. So therefore axis and their sense once you choose again the choice is arbitrary at once you

have chosen you will not change them or looking at the problems of the same crystal, okay. Well let us say I choose the 3 elections a, b, c here and that is my origin, right this is how I choose my 3 directions a, b, c the fundamental lattice transition vector would be from the origin up to the end of the unit cell that distances one unit from here to there that is one unit.

It could be 3.5 Angstrom, it could be 4.2 Angstrom depending on what space lattice it is, what is a, b what is c? It need not be 1 Angstrom, it need not be 1 centimetre, it need not be 1 millimetre mind it, it is a unit of distance along the direction a in the space lattice and that is from one lattice point to the next in that direction and that is my unit distance here. Similarly the unit distance origin to b is here unit distance from this to this is there, these are my unit distances along a, b and c, right that is important because we will be talking about these unit distances 1, 2, 3. Then in the unit cell if I had point I can always define the position coordinates of a point, so for example origin what are the position coordinates of the origin? 0, 0, 0 but my order is always a, b and c.

Let us say for example want to find out what is the position coordinates of this point let us call this point uhh x, it is going to be 1, 0, 0 that is the position coordinates. Similarly I want to find the position coordinates of this point let us call this point p, it is going to be 1, 1 and 1 those are the position coordinates of the point anywhere in the unit cell it is possible for me to find out. Let us say to find out the centre of the front face, what are the position coordinates of this along a I have to 1 along b it is half long c also it is half those are the position coordinates, is it clear? Right.

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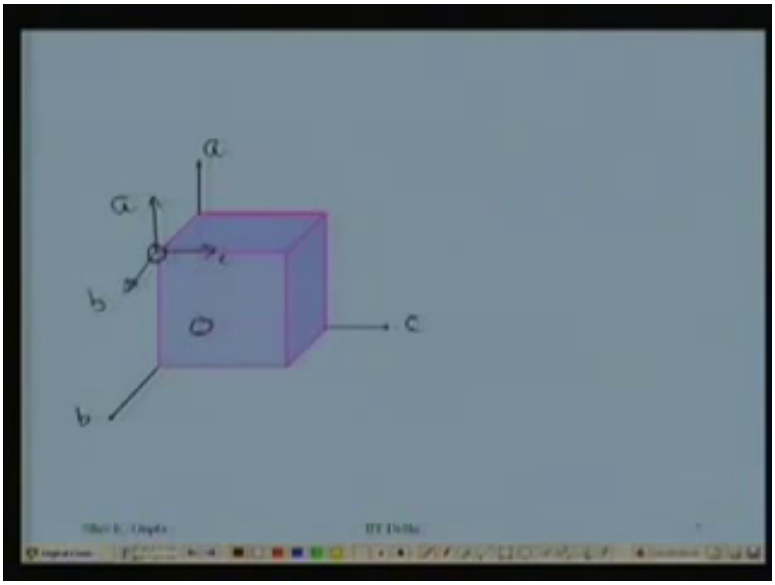

Alright now I call that a, b and c somebody can choose the origin here and call this as b, call this as a, call this as c and no (())(18:53) it can be done that is what I said sense axis you can choose arbitrary. If you require you can shift your origin from here to there in that case you will have your a going from here to there you will have your b moving in that direction and you will have your c moving in that direction, right senses not change that is the meaning of the axis once chosen the sense is not changed.

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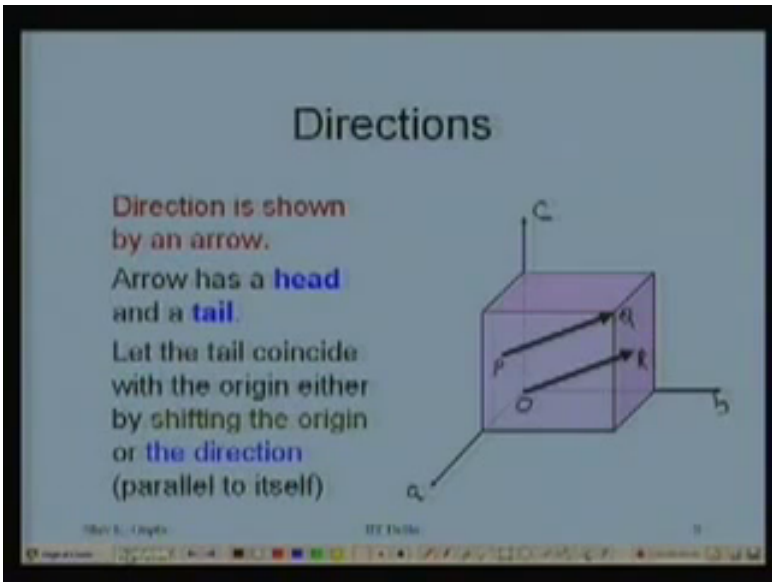

Alright let us having done that let us try to find out the Miller indices of a direction. I will show you the 2 ways in which we can work with it, I have the direction in this unit cell which is given here or let us say I am interested in finding out the name for the direction let us call it PQ I am interested in finding out with action PQ, so the one-way of doing this is let the tail coincide with the origin this can be done in 2 ways either I shift the direction parallel to itself and let it pass through the origin like the one I have shown here let us call this direction O and this is what we call it R. OR is the same direction PQ have simply has shifted parallel and passes through the origin, okay or another way is you push your origin at P to coincide with the tail of the direction arrow. Arrow has a tail and the head, so and then we can try to work out the name of this but however as I said you have to choose the uhh sense of the axis which are there let us call them a, b and c alright.

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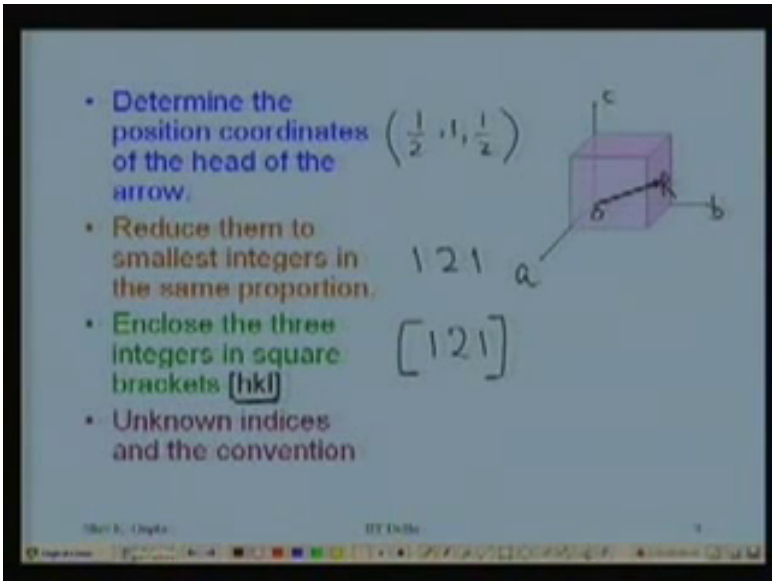

Let us go to the this is what after shifting it is, the position and I have called this as a I have called this direction a this direction b and this direction c and that is my origin. I have to determining the position coordinates of the head of the arrow, what a great position coordinates of the head of the arrow? On a you are going distance half, on b you are going distance 1 and on distance c you are going again half distance. Since the tail is at the origin reduced them to the smallest integers in the same proportion becomes 1, 2 and 1 enclose these in the square brackets where the Miller indices of this direction OR (())(22:39) that is the name of the direction OR and the crystal is 1 2 1 and unknown indices are always written as hkl you do not write xyz.

Axis we are not using xyz, indices are called hkl unknown indices and the 3 directions which choose as a, b and c other than xyz. Generally xyz you get the connotation of Cartesian system, in crystals we do not have always the Cartesian system, Cartesian system of axis will be working if I have a cube, it will not work even if I have a tetragon because a is equal to b but not equal to c, so Cartesian system is not working there. In Cartesian system ijk all 3 unit vectors are equally in magnitude, in my case they are not in crystals therefore we are using abc rather than xyz.

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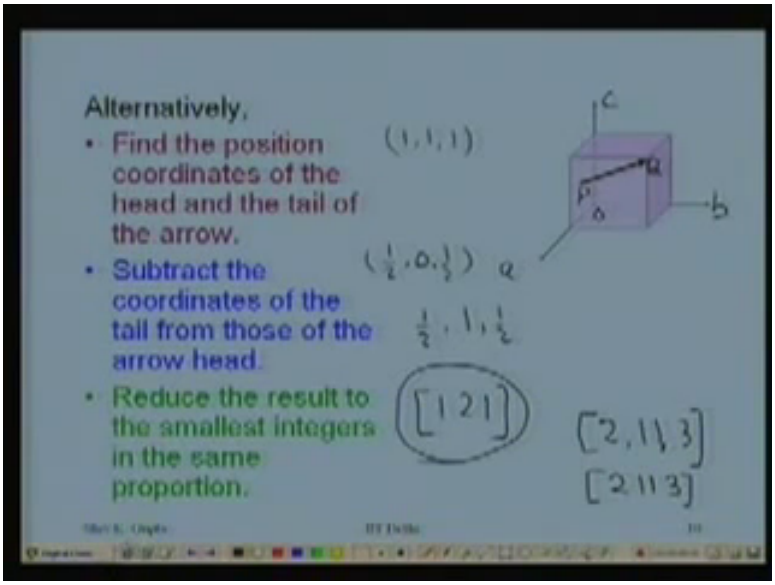

Well for the same direction again actually the direction I said was P to Q which I shifted from O to R I want to find out this direction actually. Now I do not want you to pass it to the origin or shift the origin rather I ask you to find out the position coordinates of the head, position coordinates of the tail and subtract they position coordinates of the tail from those of the head, let us see what we get?

In this case this is my origin again a, b and c, now the position coordinates of the head uhh which is Q is 1, 1, and 1 and position coordinates of the point P are half 0 and half if I subtract the position coordinate tail from those of the head I get 1 minus half is half, 1 minus 0 is 1 and 1 minus half is half and I have to convert them into integers in the same proportion and close their main square brackets I get 1, 2, 1 and here another thing which I am to say that between 1 to 1 I did not put any separator no comma no colon this is required only when I have some irrational directions which may have 2 digits say for example 2 11 3.

So if I have to ride 2 11 and 3 unless I separate them like this or I simply write it like this somebody can read it as 21 1 3 somebody can read it as 2 1 13, so to be clear we use this separator otherwise we do not use the separators when they are usually single digit, right and most of the times we have this kind of directions where we do not have to use the separators.

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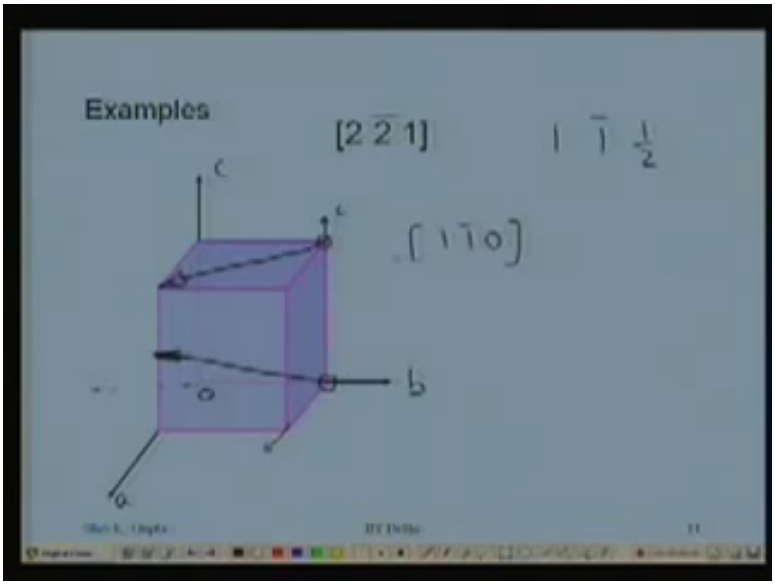

Let us look at direction 2 bar 2 1, now I have to well what is this bar business here? So far I have showed you the direction where a, b, c components were positive, now if any of the components become negative then we do not show this negative by putting minus in front of the in this index rather putting that minus on top of the index and call it bar like minus is at before the integer, here also the bar is read before the integer, so I read it as 2 bar 2 1, 2 bar 2 1 alright, so let us again use the same origin here a, b I am not changing the sense of the axis for this but now I want to know where is this direction 2 bar 2 1, firstly the unit cell cannot have any distance in terms of the position coordinates 2, it can be maximum 1, so I must reduce this indices to maximum being 1 but in the same proportion that becomes 1, minus 1 and half but these are not indices.

Starting from origin I must locate a point which have the coordinates 1, minus 1 and half. If I do that I will go or of the unit cell now minus half on be I shall have to go onto the left I will have to go out of the unit cell in this direction, so what I do is I shifted my origin without changing the sense of the axis, I keep my origin somewhere here, if I take my origin there this is the b axis, this is the a axis and this is the c axis, now let us find out the position coordinate of a point 1 minus 1 and half, 1on a is here minus half minus 1 on b will be there and plus half on c will be here that is the middle point of this axis and therefore I joint it from this to the origin and show the arrow like this that is the direction 2 bar 2 1, is it clear? Now tell me what is this direction? Now I am asking the problem the other way round have showed you an earlier example… Pardon.

Student: (())(30:07)

Look starting this if I put my origin here on a I am travelling plus 1 on b I am travelling minus 1 on c I do not travel at all, so this direction is 1 bar 1 0, good (())(30:27) so you can work out more example like that.

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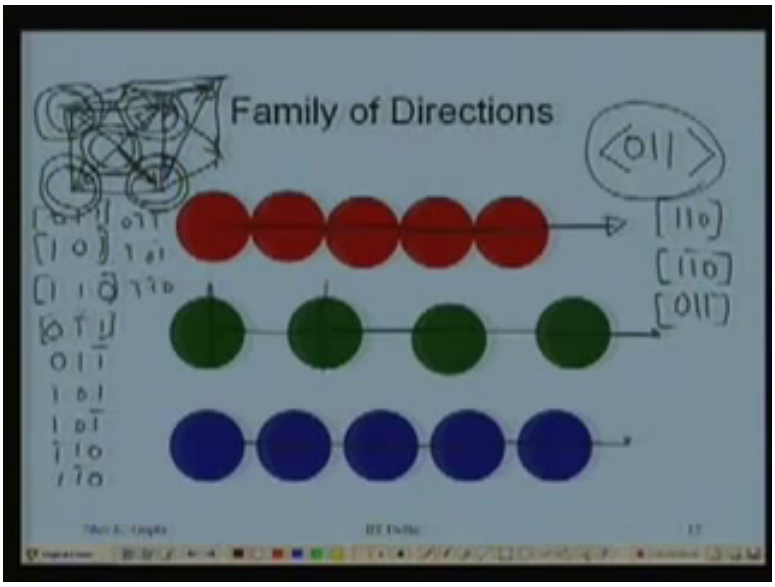

Right, then in the crystals we have family of directions, family by family what I mean is a direction which looks physically identical to another direction and not parallel to it if it is parallel is the same direction. Look physically identical but not parallel say for example I talk of a face centred cubic crystal alright, in face centred cubic crystal item look at the face diagonal, the distance between 2 atoms you will find as a minimum distances between 2 lattice points, it has the minimum distance between atoms is the diameter, it looks something like this, it looks something like this and one of the face diagonal I just showed you is of the kind 1 1 0 and the one which we have named was 1 bar 1 0, you can also find out something 0 1 1.

All this face diagonals will be looking like this, are they parallel? They are not. I will just show you again a simple… This is a cube I just show you the front face of the FCC, this is one diagonal that is another diagonal and as per the definition this is the smallest distance between the 2 neighbours, so the spears must be touching actually they must be bigger than that, okay that is how it looks like, so this direction which I am talking about the diagonal or it is this diagonal or it is that diagonal they will all look like this they all form a family then it is a family, we represent it not like this we represent it by caret and within the caret we put indices of anyone of them.

Anyone of the members I can put the indices inside the caret it represents all the family, now how many members do you think in a cube would be there which are the face diagonals. On this face I have 2 but this is an opposite one, this is an opposite one, so this will become 4 if I look all of them so there will be 12 members 4 of these, 4 on this face like this and 4 on the top face they will all look alike out of these 6 are nonparallel remaining 6 are opposite of these, why? And this if you try to expand is in a cube abc or equal abc can be permuted.

So 0 1 1 if you permute can become 1 0 1 it can become 1 1 0 that is how you have permuted 0, you can make one of them negative let us put it here can make one of them negative it is like this or like that or similarly you can make the other one or you can make in the 2nd uhh in the last one. Now you can make 2 of them negative, right is there only 2 once both of them can be made negative like this how many I have made. This one is opposite to this, this one is opposite to that, this one is opposite to this and if these are talking about the individual directions I must put the spear (())(35:55) so on and so forth, right.

This I talked about one direction there could be another direction in the same crystal let us talk about the edges of the FCC where atoms are not touching, this distances more than the diameter and since I am considering them hard spears there is space between them, this space can be small this space can be large landing on which direction am looking at, unless the direction is like this or the direction could be some space or it could be something like this. They are all different directions they will have different name characteristics of the crystals in these different directions will be different that is why there is a need for us to give them different names.

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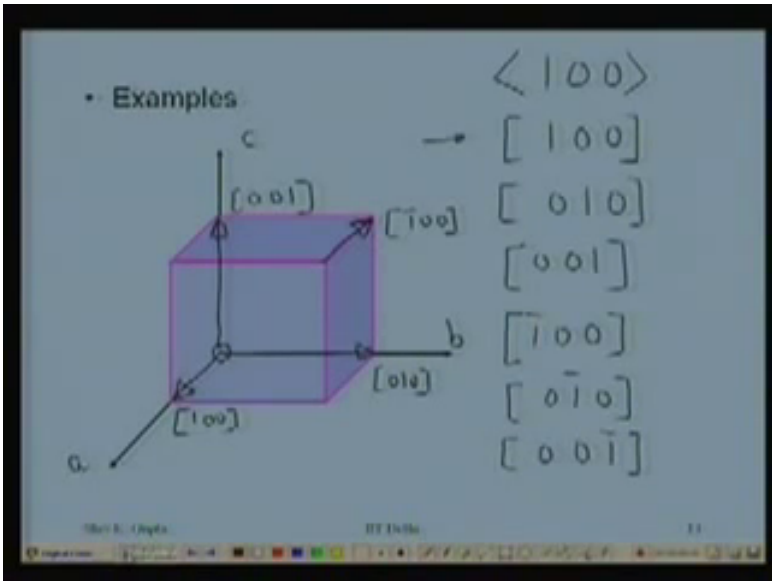

Alright, now let us have some examples of the family, I will take a simple one I have taken already one the face diagonals another example we take of a family 1 0 0 and the permutation the members are going to be 1 0 0, 0 1 0 and 0 0 1 and the opposite of these bar 1 0 0, 0 bar 1 0 and 0 0 bar 1, right. So if I again choose these as the origin that is my a axis, this is my b axis this is my c axis whereas the 1st direction 1 0 0, this is the direction 1 0 0, right where is the direction 0 1 0, this is the direction 0 1 0 and that is the direction 0 0 1. Now what is this direction we will call it bar 1 0 0 as I said bar is to be ready before the digit, if I read it 1 bar that means I am talking about the bar of the 2nd digit, so bar 1 0 0, okay. Like that you can find out the rest of them, now after having uhh look at the directions, the families of direction we shall look at the plains geometrical plains and the crystal.

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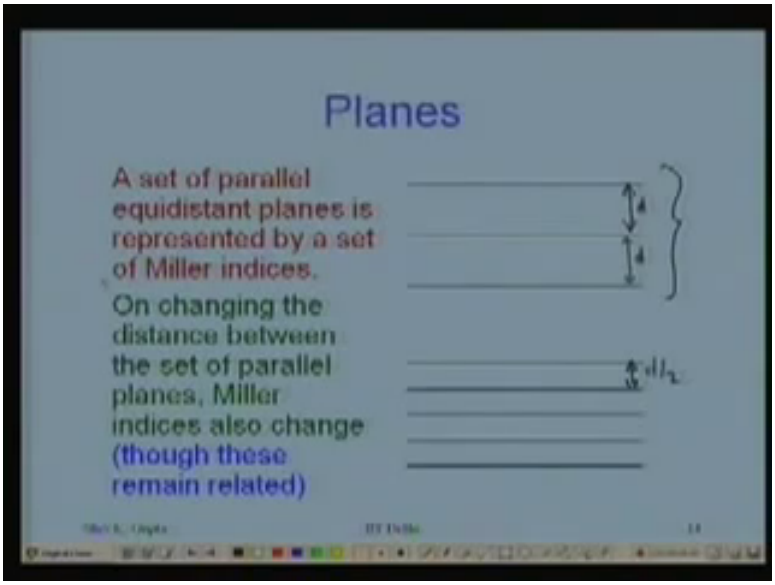

In case of planes like in case of direction a set of equidistant planes uhh a set of equidistant parallel planes, so equidistant the whole set is a set of parallel planes and they are at the same time equidistant like say for example I talk of this set in a given crystal, this set and the distance between the consecutive planes is let us say is d that distance is same into the next but here the same set parallel in the same crystal but the distance is different, let us say it is d by 2, so this said and this set will have slightly different name though they will be maybe related names but they will be different. Set of parallel to distant planes is represented by set of Miller indices, these are also called Miller indices, okay and of course on changing the distance is assured here the name can change but if they are parallel to the name would be related, okay.

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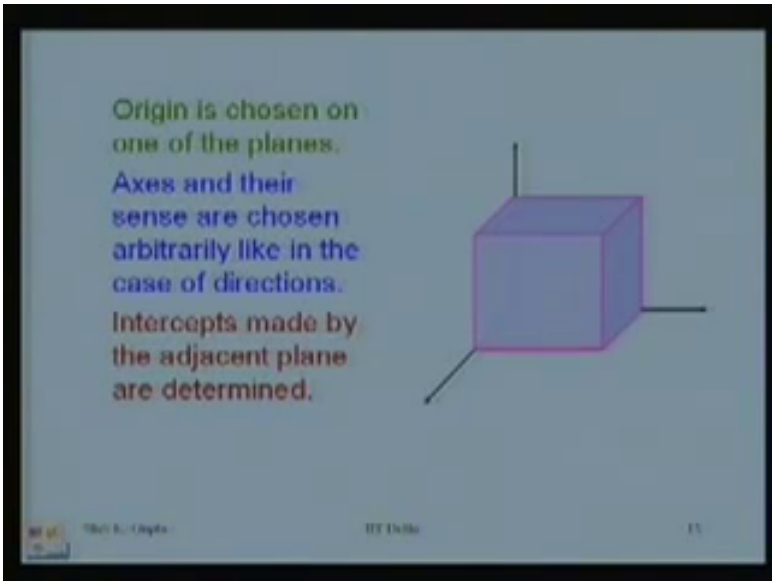

Now for doing this what we do is again we choose the origin in the refer to unit cell again choose the axis and their sense and the choice is arbitrary and then what we work out are the intercepts made by the adjacent planes house origin is taken on one planes.

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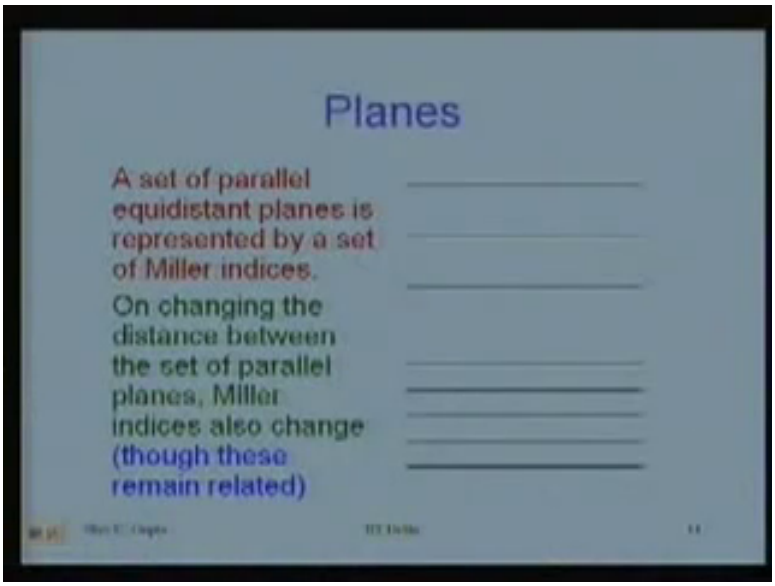

Say for example here there are 3 planes 1, 2 and 3 I choose the origin on the middle plane then I find out the uhh after making the axis in the crystal what are the intercepts made by this plane on those three axis or if I have chosen the origin here I find out the intercepts made by this plane, right there will be slight difference in the name and we find out for this one and that one because once the origin is here and the axis have been chosen if the intercepts made by this is plus 1, intercepts made by that one will be minus 1, so if there is a plane hkl this

one is named as hkl this one would be named bar h bar k bar l but in our mind we know it is we are talking about the same set of planes one is on one side of the origin other one is on the other side of the origin and origin is taken on one plane, okay but I cannot find out the indices of the plane on which I have chosen the origin because the plane is passing through the origin it is not possible for me to find out the intercepts made by it on a axis, b axis and c axis is not possible, is that clear?

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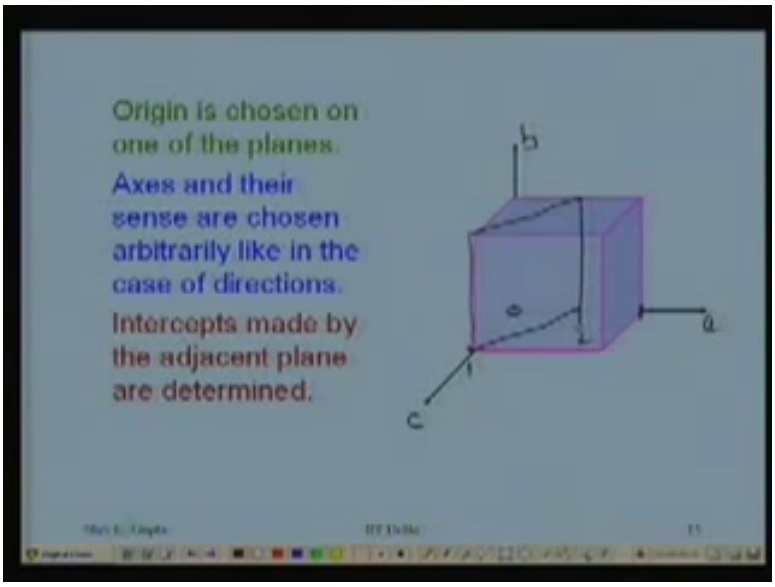

So that is what uhh we are going to do, so intercept made by the adjacent lane are determined, right. Alright let me choose a plane here and then we shall try to find out its intercepts okay the plane let me choose is… In the crystal this is a plane alright and I choose my origin here let us call this as the a axis now let me change my sense of the axis b here and let us call this one c. I want to find out the intercepts made by this plane on a b and c, right. Alright so how do you go about doing that, that is my origin, intercept made by this plane on the a axis is how much 1 by 2, okay unit is again from 0 to 1 here. What is the intercept made by it on the b axis, b axis lie on the plane it goes up to infinity, so it meets at plane at the infinity, okay. So the intercept made on the b axis is infinity and what is the intercept made on the c axis? 1 so this is half this is one and there it goes parallel, alright so let us go and see how we name this plane.

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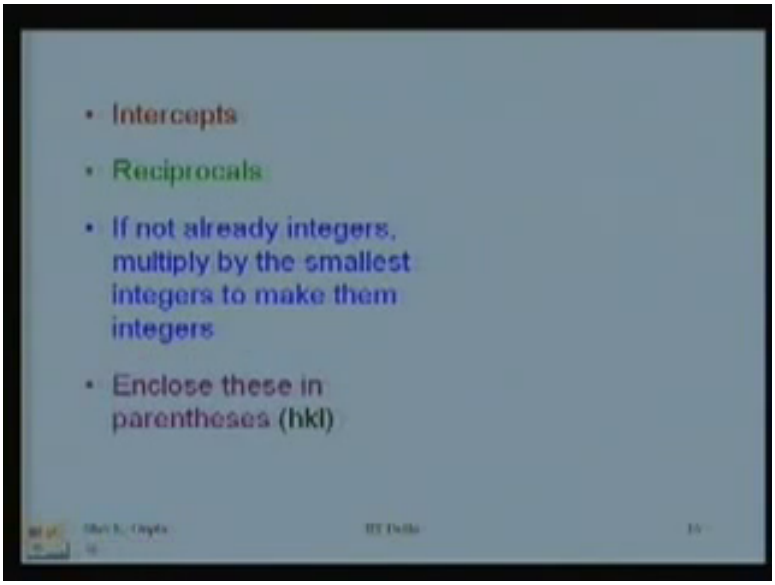

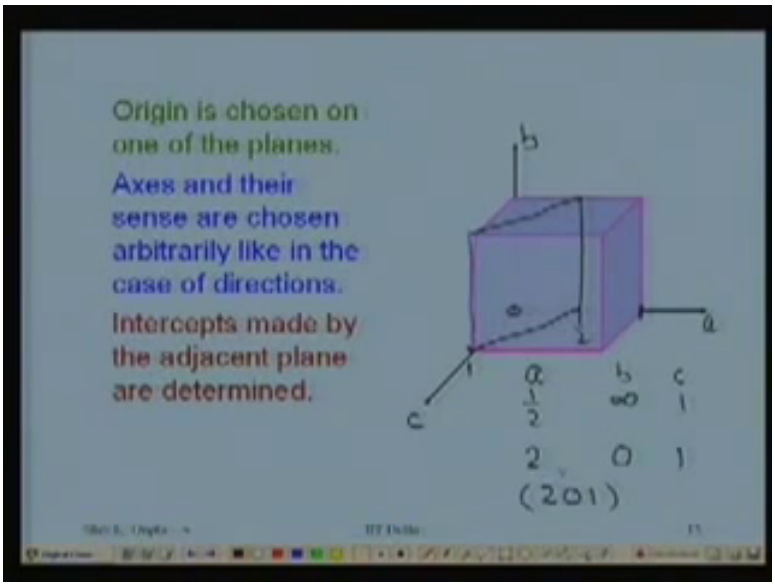

Now once I found out the intercepts made again we write the order is same the axis 1st, b axis and then c axis, so all are (())(45:15). Alright so the 3 axis let us write down a b and c in that order on a we found out the intercept to be half and on b the intercept we found it to be infinity on the c the intercept we found it to be 1. 2nd step is we have to take the reciprocals, reciprocal of half is 2 reciprocal of infinity is 0 and reciprocal of 1 is 1. If these are integers we do not do anything about it, if these are not integers we multiply by an integer to make them integers and you multiply by this small possible integer which you can find out by taking the (())(46:55), okay and then this are closed in parenthesis that is the name of this plane which I have chosen 2 0 1, is that right? Name this plane as 2 0 1 alright but this is may be an example for us to see the Miller indices of this plane let us do that.

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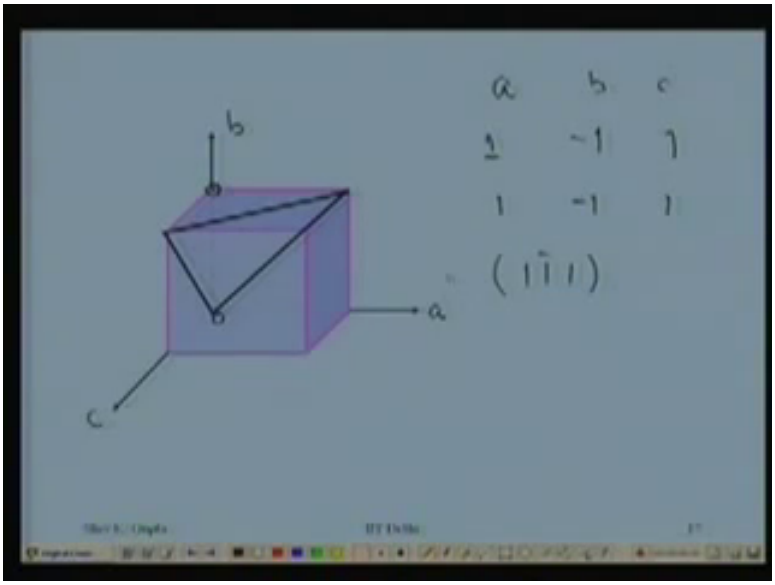

I choose my origin again here let us call this as the what we call this uhh a axis we call here, we call this as b axis we call this as the c axis alright now this is the plane which is chosen assess through the origin, so I am a ship the origin to another plane parallel to it, okay. So therefore let us take the origin uhh here, shift the origin sense of the axis is not changed, so what intercepts does it make on a b and c now let us see from starting from the origin this plane intercepts the a axis on plus 1, starting from this origin on the b it intercept here which is minus 1. Starting from this origin on c it intercepts here which is plus 1 reciprocals one minus 1 and 1 are the reciprocals these are already integers and minus will be capped on top and read as it is 1 bar 1 1 and closing parenthesis, right.

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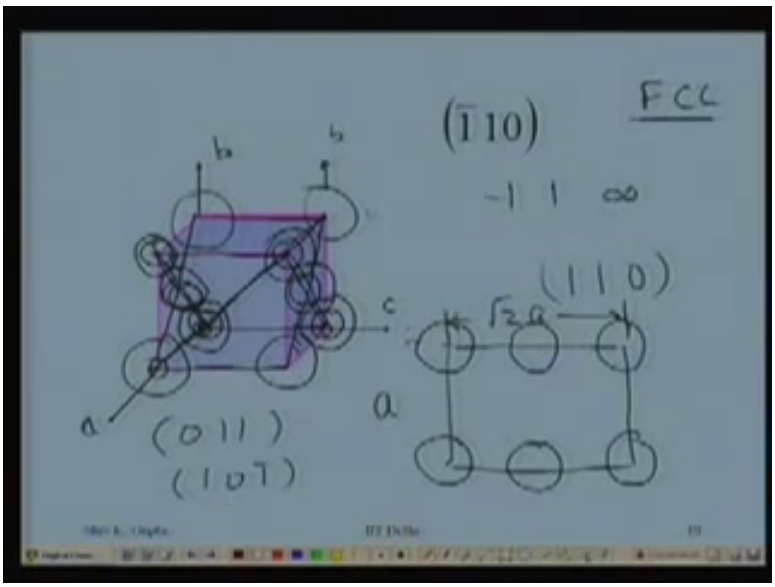

Alright next example is put is now the plane is given to you bar 1 1 0 name is given you have to locate this again let us choose the origin axis again let a b and c if it is not the same crystal it is a different crystal you can always change the axis alright but let us consider the same unit cell bar 1 1 0 now what have to do is I have 2 1st take the reciprocals of the indices I am going to opposite direction now, reciprocal of this is minus 1 reciprocal is one and 0 is infinity. I have to make the intercepts minus 1 on a, 1 on b and infinity on c, when the plane is going to go parallel to the c alright so starting from the origin if I take minus 1 on a I have to go out so I shift my origin from here to there then minus 1 on a the intercept is here plus 1 on b the intercept this here because b axis is going to be here that is going to be b, so these are the 2 intercepts and it is going to run parallel to c.

So join these 2 intercepts and run parallel to c from there. I am sorry this is turn out to be just a line this whole plane while you see that this plane is possible for me to show you much better than this if I change the change the sense of the axis or the axis themselves, say for example uhh I name let us call this one as c and this one as a let us make this change. Now if I do this my origin will be here minus 1 intercept on a I shall go there plus 1 intercept on b I shall go here and parallel to c I have to run to join these intercepts sorry run parallel to c from here I am sorry I have to rub few lines here I can rub okay that is the plane I have, right so this is the plane now you can see that plane or earlier it was just becoming a line you were not able to see that because of the cube the way it has been drawn.

So this is depends upon how we are viewing it that is what we go about catching the plane and that is bar 1 1 0 plane in the unit cell like we had the family of directions in the crystal we also have family of planes there could be sets of parallel planes which are equidistant but not parallel to each other but differently oriented in space in the crystal and then looking like or I proceed there let me just talk about this in itself bar 1 1 0 and in this bar 1 1 0 let us talk about an FCC one atom is here another atom is here in FCC and this is the face centres if I make them little bigger one they can be made to touch like this.

So these are the arrangement of atoms in the bar 1 1 0 plane in FCC. Similarly let us look at a plane in the same unit cell this 1 1 0 which is 1 1 0 here intercepts by 1 on a 1 on b infinity on c again intercepts starting from this origin 1 is a here 1 is b there so it will be a plain like this. In here the atoms are arranged beside this face center they are arranged here, so if I look at the 2 planes both the planes look like this, this distances is equal to lattice parameter a this distance is a face diagonal equal to under root 2 of a is a rectangle and atoms are arranged

these locations sorry, for the reason for clarity I am not making them uhh touch otherwise they will become very clumsy, so this is the arrangement whether is a bar 1 1 0 plane or it is a 1 1 0 plane you will see the same story if the plane is 0 1 1 or the plane is 1 0 bar 1 or any other member of the family. This is what we call a family they are not parallel but the arrangement of atom is same the physically identical plane, so characteristics of the crystal on these planes will be similar.

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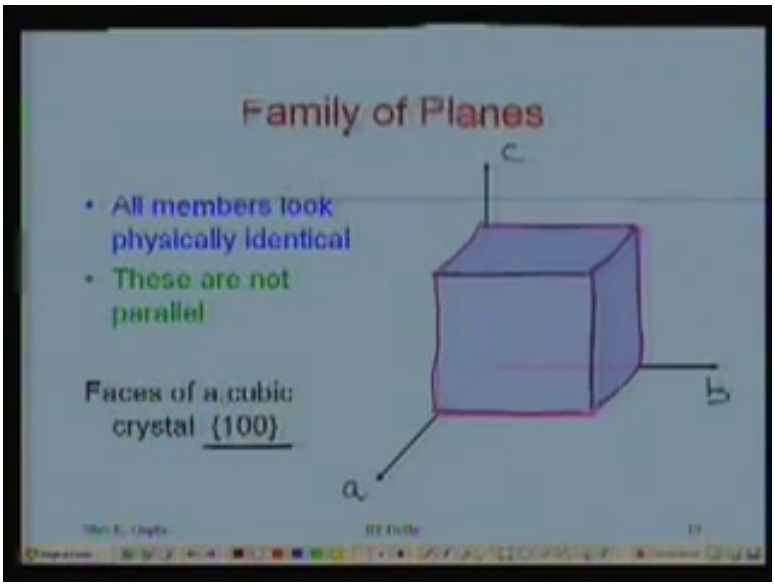

So family of planes is what we call them and this family of planes by uhh the curly bracket or braces right let a over this family 1 0 0 again this is my direction a, direction c, direction c. 1 0 0 is the front face is the another member would be 0 1 0, 0 1 0 is this right hand side face. Another member would be 0 0 1 (())(56:23) similarly would have other member bar 1 0 0 the backspace you will have the members 0 bar 1 0 in the left-hand side face you would have 0 0 bar 1 bottom face, okay. All the 6 faces form a member in all form a (())(56:47) and not parallel you can see that. Only 1 (())(56:53) 0 0 is parallel to bar 1 0 0 and that I told you. One is taken the one side of the origin other is taken on the other side of the origin, so we are talking about the same set of (())(57:04).

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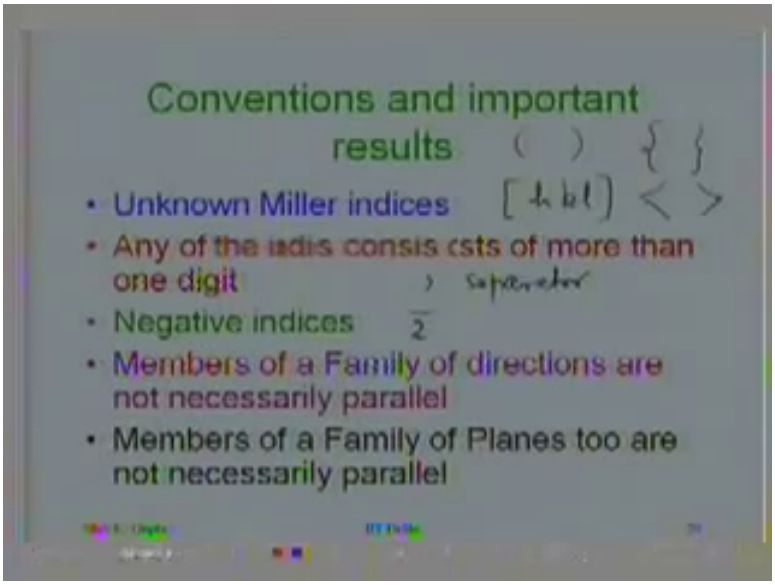

Right now quickly we will revise what we have talked about unknown Miller indices are (()) (57:24) as hkl for single direction (())(57:31) brackets for family of direction we use caret for planes we use parenthesis and for a family of planes we use basis. Well we only when one of the index happens to be of 2 digits we use a separator may be a comma otherwise separator is not used. Negative indices we put the bar on top and read it as bar 2. Members of the family of direction are not necessarily parallel and similarly members of a family of planes to are not necessarily parallel, okay.

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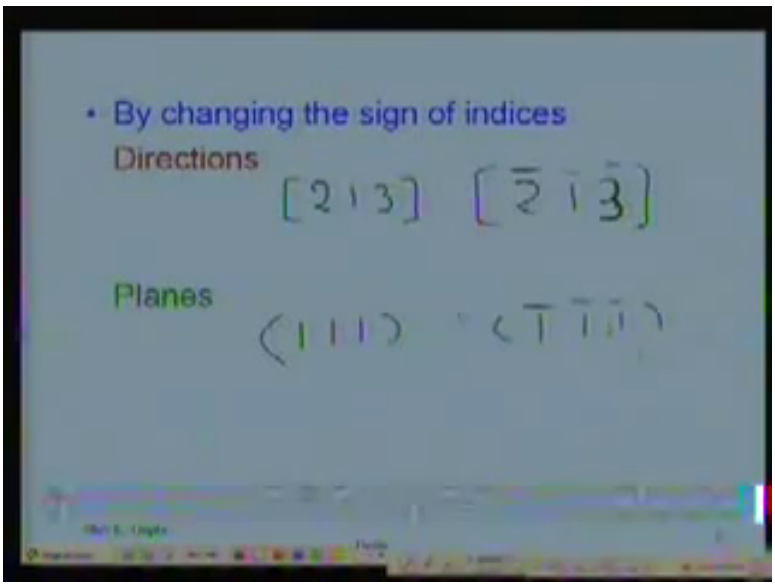

By changing the sign of indices we can change the direction opposite to each other say for example I have just given the example of a direction let us say 2 1 3 and I have bar 2 bar 1

bar 3 is opposite to this, right similarly planes by changing the signs it is the same set is not different but only thing is one is on one side of the origin other is on the other side of the origin that is let us talk about 1 1 1 and the other one is bar 1 bar 1 bar 1 they are parallel, right, alright so will stop here.